



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2022 – 02:07 PM EST

PDB ID : 7LBW  
Title : Crystal structure of TFAM (mitochondrial transcription factor A) bridging two non-sequence specific DNA substrates  
Authors : Choi, W.S.; Garcia-Diaz, M.  
Deposited on : 2021-01-09  
Resolution : 2.84 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.25  
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) : 2.25

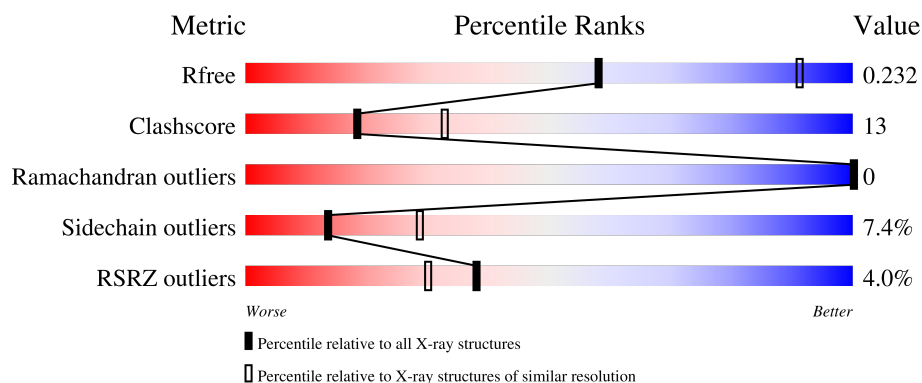
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

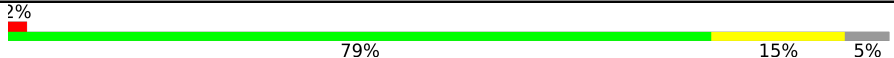
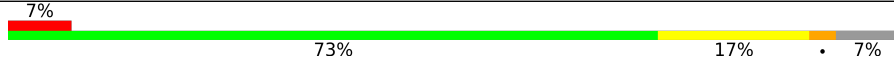



The reported resolution of this entry is 2.84 Å.

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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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  $\geq 3$ , 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	204	
1	B	204	
2	C	22	
2	E	22	
3	D	22	

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Mol	Chain	Length	Quality of chain
3	F	22	

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
4	EDO	B	303	-	-	-	X
4	EDO	C	101	-	-	X	-
5	PEG	B	305	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5258 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 Transcription factor A, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	1	0
			1625	1027	291	301	6			
1	B	190	Total	C	N	O	S	0	0	0
			1598	1009	288	295	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	P	0	0	0
			433	206	70	136	21			
2	E	22	Total	C	N	O	P	0	0	0
			434	207	70	136	21			

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

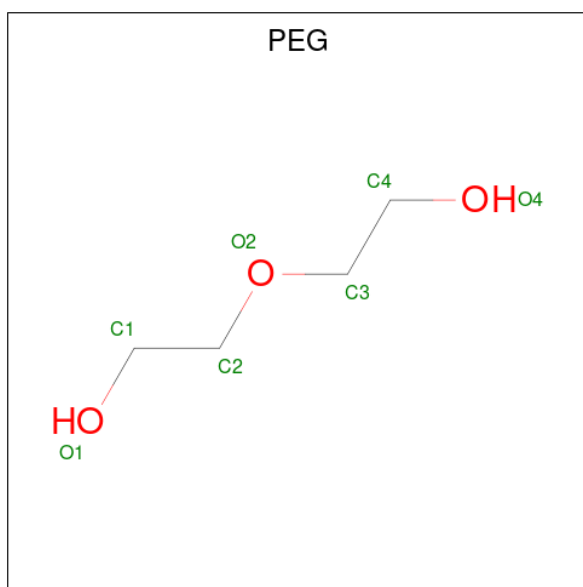
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	22	Total	C	N	O	P	0	0	0
			450	213	92	124	21			
3	F	22	Total	C	N	O	P	0	0	0
			450	213	92	124	21			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

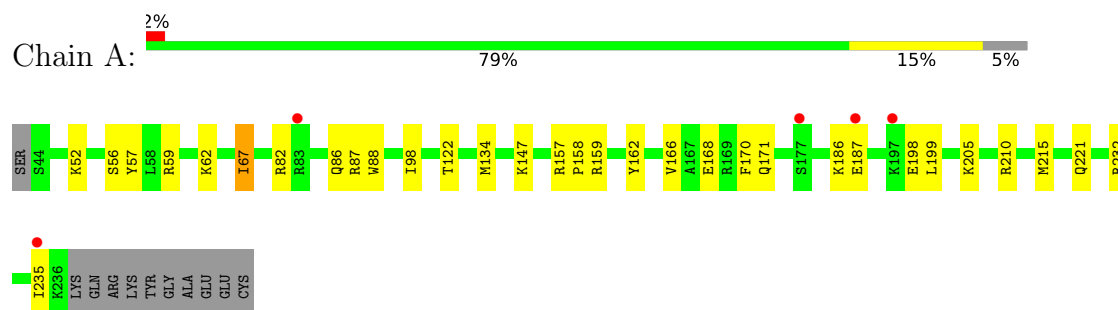
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	74	Total	O	0	0
			74	74		
6	B	72	Total	O	0	0
			72	72		
6	C	14	Total	O	0	0
			14	14		
6	D	16	Total	O	0	0
			16	16		
6	E	8	Total	O	0	0
			8	8		
6	F	39	Total	O	0	0
			39	39		

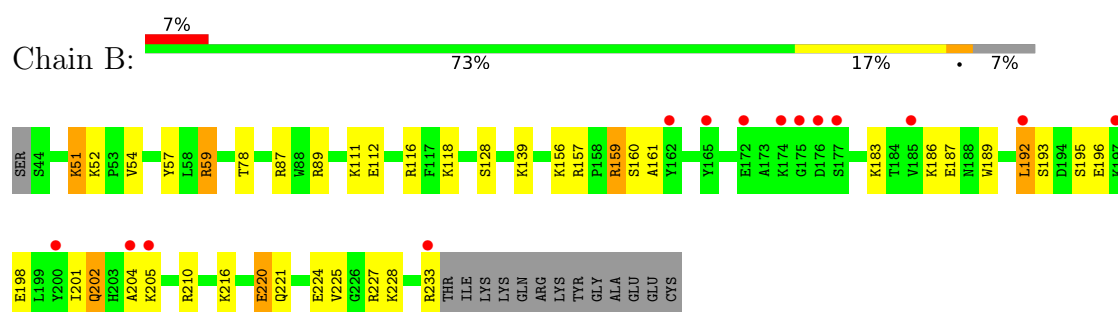
### 3 Residue-property plots [i](#)

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: Transcription factor A, mitochondrial



- Molecule 1: Transcription factor A, mitochondrial



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

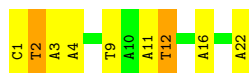


- Molecule 2: DNA (5'-D(P\*TP\*AP\*GP\*CP\*CP\*TP\*TP\*TP\*CP\*TP\*AP\*TP\*TP\*AP\*GP\*C P\*TP\*CP\*TP\*TP\*AP\*G)-3')



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

Chain D:  59% 32% 9%



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

Chain F:  59% 32% 9%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.00Å 124.81Å 55.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 2.84 39.81 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.81-2.84) 99.9 (39.81-2.84)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.65 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, BUSTER	Depositor
R, $R_{free}$	0.199 , 0.232 0.198 , 0.232	Depositor DCC
$R_{free}$ test set	996 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.1	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5258	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, PEG

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	0.51	0/1656	0.65	0/2217
1	B	0.50	0/1629	0.62	0/2180
2	C	1.16	0/483	1.03	1/739 (0.1%)
2	E	1.10	0/484	1.03	1/741 (0.1%)
3	D	1.11	0/508	1.04	1/781 (0.1%)
3	F	1.17	1/508 (0.2%)	1.03	1/781 (0.1%)
All	All	0.80	1/5268 (0.0%)	0.82	4/7439 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	5
2	E	0	6
3	D	0	3
3	F	0	3
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	DC	C1'-N1	5.28	1.56	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	DT	P-O3'-C3'	7.18	128.32	119.70
3	D	11	DA	P-O3'-C3'	7.10	128.22	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	11	DA	P-O3'-C3'	6.95	128.04	119.70
2	C	8	DT	P-O3'-C3'	6.33	127.30	119.70

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1	DT	Sidechain
2	C	10	DT	Sidechain
2	C	17	DT	Sidechain
2	C	7	DT	Sidechain
2	C	8	DT	Sidechain
3	D	12	DT	Sidechain
3	D	2	DT	Sidechain
3	D	9	DT	Sidechain
2	E	1	DT	Sidechain
2	E	10	DT	Sidechain
2	E	17	DT	Sidechain
2	E	6	DT	Sidechain
2	E	7	DT	Sidechain
2	E	8	DT	Sidechain
3	F	12	DT	Sidechain
3	F	2	DT	Sidechain
3	F	9	DT	Sidechain

## 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	1625	0	1659	34	1
1	B	1598	0	1632	53	0
2	C	433	0	227	10	0
2	E	434	0	230	5	0
3	D	450	0	236	14	0
3	F	450	0	236	9	0
4	A	8	0	12	3	0
4	B	12	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	4	0	6	11	0
5	A	7	0	9	0	0
5	B	14	0	16	4	0
6	A	74	0	0	24	2
6	B	72	0	0	44	1
6	C	14	0	0	3	0
6	D	16	0	0	13	0
6	E	8	0	0	4	0
6	F	39	0	0	6	0
All	All	5258	0	4281	124	2

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 13.

All (124) 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:B:157:ARG:HB2	6:D:104:HOH:O	1.29	1.30
1:B:221:GLN:HG2	6:B:408:HOH:O	1.40	1.17
1:A:235:ILE:HD11	6:A:444:HOH:O	1.50	1.09
1:A:67:ILE:CD1	6:A:463:HOH:O	2.00	1.06
2:C:15:DG:H5'	4:C:101:EDO:O1	1.57	1.05
6:B:419:HOH:O	3:F:11:DA:H5'	1.61	1.00
1:A:157:ARG:HD2	6:A:405:HOH:O	1.59	1.00
1:B:204:ALA:HB1	6:B:404:HOH:O	1.63	0.97
1:A:67:ILE:HD13	6:A:463:HOH:O	1.64	0.94
1:A:147:LYS:HE2	6:D:109:HOH:O	1.65	0.94
2:E:15:DG:H5'	6:E:106:HOH:O	1.67	0.93
2:C:15:DG:C5'	4:C:101:EDO:O1	2.16	0.92
1:B:202:GLN:HG3	6:B:409:HOH:O	1.69	0.92
3:D:16:DA:H5'	6:D:104:HOH:O	1.70	0.90
1:B:59:ARG:HB2	6:B:450:HOH:O	1.71	0.90
1:B:57:TYR:HB3	6:F:104:HOH:O	1.73	0.88
3:D:2:DT:H1'	6:D:107:HOH:O	1.75	0.86
1:A:82:ARG:HD2	6:A:452:HOH:O	1.75	0.86
1:B:160:SER:HA	6:B:404:HOH:O	1.77	0.84
2:C:14:DA:H1'	6:C:211:HOH:O	1.78	0.84
3:D:4:DA:H5'	6:D:109:HOH:O	1.76	0.83
1:B:228:LYS:HE2	6:B:460:HOH:O	1.76	0.83
1:B:52:LYS:HG3	4:C:101:EDO:H22	1.60	0.82
6:B:419:HOH:O	3:F:10:DA:H4'	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:MET:CE	6:A:437:HOH:O	2.31	0.79
3:F:12:DT:H6	6:F:117:HOH:O	1.65	0.78
1:B:52:LYS:HD2	6:B:467:HOH:O	1.81	0.78
1:B:52:LYS:HG3	6:B:428:HOH:O	1.84	0.77
1:B:187:GLU:CG	6:B:403:HOH:O	2.31	0.77
3:F:13:DA:H1'	6:F:113:HOH:O	1.86	0.75
1:B:225:VAL:CG1	6:B:463:HOH:O	2.34	0.75
1:A:56:SER:HB2	6:A:442:HOH:O	1.85	0.75
1:B:204:ALA:CB	6:B:404:HOH:O	2.29	0.73
1:B:187:GLU:HG3	6:B:403:HOH:O	1.87	0.72
1:B:52:LYS:CG	6:B:428:HOH:O	2.36	0.72
1:B:51:LYS:HG2	4:C:101:EDO:H11	1.72	0.71
1:B:227:ARG:HD3	6:B:441:HOH:O	1.90	0.71
1:B:228:LYS:CE	6:B:460:HOH:O	2.36	0.70
3:D:2:DT:O4'	6:D:101:HOH:O	2.08	0.70
1:A:67:ILE:HA	6:A:429:HOH:O	1.90	0.70
3:D:1:DC:H2''	6:D:101:HOH:O	1.92	0.70
1:A:168:GLU:HB3	6:A:412:HOH:O	1.90	0.70
2:E:14:DA:H8	6:E:104:HOH:O	1.76	0.68
1:A:86:GLN:CB	6:A:403:HOH:O	2.41	0.67
5:B:305:PEG:H32	6:B:436:HOH:O	1.94	0.67
1:A:235:ILE:H	4:A:302:EDO:C1	2.08	0.67
1:B:116:ARG:HB2	4:B:302:EDO:O2	1.94	0.66
1:B:161:ALA:N	6:B:404:HOH:O	2.28	0.66
1:B:202:GLN:CG	6:B:409:HOH:O	2.35	0.66
2:E:5:DC:H5'	6:E:102:HOH:O	1.96	0.65
3:D:1:DC:C2'	6:D:101:HOH:O	2.44	0.65
1:B:87:ARG:NH1	6:B:405:HOH:O	2.28	0.65
1:B:51:LYS:HG2	4:C:101:EDO:C1	2.27	0.64
1:A:235:ILE:H	4:A:302:EDO:H11	1.61	0.64
1:B:156:LYS:NZ	6:B:406:HOH:O	2.31	0.63
3:D:2:DT:H5'	6:D:101:HOH:O	1.97	0.63
1:A:57:TYR:HB3	6:A:409:HOH:O	1.97	0.62
1:A:157:ARG:NH1	6:A:405:HOH:O	2.27	0.61
1:B:128:SER:HB2	6:B:432:HOH:O	1.99	0.61
3:F:11:DA:H3'	6:F:110:HOH:O	2.01	0.61
2:C:15:DG:H5''	4:C:101:EDO:O1	1.98	0.60
3:F:15:DA:H1'	6:F:102:HOH:O	2.02	0.59
1:B:118:LYS:NZ	6:B:407:HOH:O	2.35	0.59
1:B:156:LYS:HB2	1:B:159:ARG:HH21	1.67	0.59
1:B:225:VAL:HG12	6:B:463:HOH:O	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221[A]:GLN:NE2	6:A:408:HOH:O	2.35	0.57
1:B:220:GLU:HG2	6:B:455:HOH:O	2.04	0.57
1:A:232:ARG:CZ	1:A:235:ILE:HG23	2.35	0.56
1:B:221:GLN:CG	6:B:408:HOH:O	2.18	0.56
3:D:12:DT:H6	6:D:108:HOH:O	1.88	0.56
1:A:86:GLN:HB2	6:A:403:HOH:O	2.04	0.56
1:B:89:ARG:NH2	6:B:411:HOH:O	2.39	0.56
2:C:14:DA:H2''	4:C:101:EDO:O2	2.05	0.56
5:B:305:PEG:H22	6:B:436:HOH:O	2.07	0.55
5:B:305:PEG:C3	6:B:436:HOH:O	2.53	0.55
1:B:59:ARG:CB	6:B:450:HOH:O	2.40	0.54
1:B:160:SER:CA	6:B:404:HOH:O	2.46	0.53
1:A:134:MET:HE1	6:A:437:HOH:O	2.02	0.53
1:B:52:LYS:HG2	6:B:428:HOH:O	2.06	0.52
1:B:220:GLU:CB	6:B:455:HOH:O	2.58	0.52
1:B:160:SER:C	6:B:404:HOH:O	2.48	0.51
1:A:215:MET:HE1	6:A:430:HOH:O	2.09	0.51
2:E:8:DT:H2''	2:E:9:DC:O5'	2.11	0.51
1:B:52:LYS:HB2	6:B:467:HOH:O	2.12	0.50
1:A:82:ARG:CD	6:A:452:HOH:O	2.46	0.49
1:B:111:LYS:HD2	6:B:459:HOH:O	2.12	0.49
1:B:189:TRP:O	1:B:192:LEU:HB2	2.12	0.49
1:B:186:LYS:NZ	6:B:403:HOH:O	2.23	0.49
5:B:305:PEG:C2	6:B:436:HOH:O	2.61	0.48
3:D:3:DA:H1'	6:D:109:HOH:O	2.12	0.48
2:C:8:DT:H2''	2:C:9:DC:O5'	2.12	0.48
1:B:187:GLU:CD	6:B:403:HOH:O	2.52	0.47
1:B:112:GLU:HG3	4:B:302:EDO:H11	1.97	0.47
1:A:166:VAL:O	1:A:170:PHE:HB2	2.14	0.47
3:D:22:DA:C2	2:E:2:DA:C2	3.02	0.47
1:A:147:LYS:HA	6:C:202:HOH:O	2.15	0.46
1:B:52:LYS:HG3	4:C:101:EDO:C2	2.40	0.46
1:A:162:TYR:O	1:A:166:VAL:HG23	2.15	0.46
1:A:235:ILE:H	4:A:302:EDO:H12	1.79	0.46
1:A:52:LYS:HG3	6:A:468:HOH:O	2.15	0.46
1:B:52:LYS:HE2	4:C:101:EDO:C2	2.46	0.45
1:B:52:LYS:HE2	4:C:101:EDO:H21	1.97	0.45
2:C:15:DG:H5'	4:C:101:EDO:HO1	1.73	0.45
1:A:122:THR:CB	6:A:401:HOH:O	2.60	0.45
1:A:199:LEU:CD2	6:A:414:HOH:O	2.64	0.45
2:C:2:DA:C2	3:F:22:DA:C2	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:GLU:HA	1:B:201:ILE:HB	1.97	0.45
2:C:1:DT:C5'	6:C:202:HOH:O	2.65	0.44
1:B:118:LYS:HD2	6:B:413:HOH:O	2.19	0.42
1:B:220:GLU:CG	6:B:455:HOH:O	2.65	0.42
3:F:15:DA:N3	6:F:102:HOH:O	2.37	0.42
1:B:52:LYS:CB	6:B:467:HOH:O	2.68	0.42
1:B:220:GLU:HB2	6:B:455:HOH:O	2.18	0.42
1:B:139:LYS:HE3	6:E:105:HOH:O	2.19	0.42
1:A:98:ILE:O	6:A:402:HOH:O	2.21	0.42
3:D:2:DT:C5'	6:D:101:HOH:O	2.61	0.42
3:D:1:DC:H2'	6:D:101:HOH:O	2.13	0.41
1:A:158:PRO:HD2	6:A:445:HOH:O	2.19	0.41
1:A:159:ARG:NH2	6:A:418:HOH:O	2.53	0.41
1:A:52:LYS:CD	3:D:12:DT:OP1	2.69	0.41
3:D:1:DC:O4'	3:F:22:DA:H2''	2.20	0.41
1:B:54:VAL:HG12	2:C:15:DG:H2''	2.03	0.40
1:A:162:TYR:CB	6:A:417:HOH:O	2.68	0.40
1:A:86:GLN:C	1:A:88:TRP:N	2.74	0.40

All (2) 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)
6:A:452:HOH:O	6:B:462:HOH:O[4_455]	1.28	0.92
1:A:221[B]:GLN:OE1	6:A:401:HOH:O[1_556]	2.15	0.05

## 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	192/204 (94%)	187 (97%)	5 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	188/204 (92%)	186 (99%)	2 (1%)	0	100	100
All	All	380/408 (93%)	373 (98%)	7 (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	178/188 (95%)	168 (94%)	10 (6%)	21	40
1	B	175/188 (93%)	159 (91%)	16 (9%)	9	19
All	All	353/376 (94%)	327 (93%)	26 (7%)	13	29

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	62	LYS
1	A	67	ILE
1	A	87	ARG
1	A	171	GLN
1	A	186	LYS
1	A	187	GLU
1	A	198	GLU
1	A	205	LYS
1	A	210	ARG
1	B	51	LYS
1	B	59	ARG
1	B	78	THR
1	B	159	ARG
1	B	183	LYS
1	B	192	LEU
1	B	193	SER
1	B	195	SER

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Mol	Chain	Res	Type
1	B	196	GLU
1	B	202	GLN
1	B	205	LYS
1	B	210	ARG
1	B	216	LYS
1	B	220	GLU
1	B	224	GLU
1	B	233	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

9 ligands are modelled in this entry.

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	A	302	-	3,3,3	0.68	0	2,2,2	0.78	0
5	PEG	A	303	-	6,6,6	0.90	0	5,5,5	0.63	0
4	EDO	A	301	-	3,3,3	0.68	0	2,2,2	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	B	301	-	3,3,3	0.67	0	2,2,2	0.79	0
4	EDO	B	303	-	3,3,3	0.11	0	2,2,2	0.12	0
4	EDO	B	302	-	3,3,3	0.67	0	2,2,2	0.78	0
5	PEG	B	305	-	6,6,6	0.83	0	5,5,5	0.57	0
4	EDO	C	101	-	3,3,3	0.11	0	2,2,2	0.02	0
5	PEG	B	304	-	6,6,6	1.13	0	5,5,5	0.74	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	A	302	-	-	1/1/1/1	-
5	PEG	A	303	-	-	3/4/4/4	-
4	EDO	A	301	-	-	0/1/1/1	-
4	EDO	B	301	-	-	1/1/1/1	-
4	EDO	B	303	-	-	1/1/1/1	-
4	EDO	B	302	-	-	1/1/1/1	-
5	PEG	B	305	-	-	1/4/4/4	-
4	EDO	C	101	-	-	1/1/1/1	-
5	PEG	B	304	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	303	PEG	O2-C3-C4-O4
5	B	304	PEG	O1-C1-C2-O2
5	B	305	PEG	O1-C1-C2-O2
4	B	302	EDO	O1-C1-C2-O2
5	A	303	PEG	O1-C1-C2-O2
5	A	303	PEG	C4-C3-O2-C2
4	B	303	EDO	O1-C1-C2-O2
4	C	101	EDO	O1-C1-C2-O2
4	A	302	EDO	O1-C1-C2-O2
4	B	301	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302	EDO	3	0
4	B	302	EDO	2	0
5	B	305	PEG	4	0
4	C	101	EDO	11	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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	193/204 (94%)	0.29	5 (2%)	56	51	44, 68, 108, 129	0
1	B	190/204 (93%)	0.46	14 (7%)	14	9	46, 69, 141, 164	0
2	C	22/22 (100%)	-0.31	0	100	100	51, 80, 106, 107	0
2	E	22/22 (100%)	-0.21	0	100	100	83, 95, 113, 121	0
3	D	22/22 (100%)	-0.08	0	100	100	78, 95, 117, 121	0
3	F	22/22 (100%)	-0.13	0	100	100	49, 66, 106, 139	0
All	All	471/496 (94%)	0.27	19 (4%)	38	30	44, 72, 124, 164	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	TYR	3.5
1	B	176	ASP	3.4
1	B	174	LYS	3.4
1	B	204	ALA	3.3
1	B	177	SER	3.0
1	B	192	LEU	2.9
1	A	235	ILE	2.8
1	B	200	TYR	2.7
1	B	197	LYS	2.7
1	B	205	LYS	2.6
1	B	233	ARG	2.4
1	B	162	TYR	2.4
1	B	172	GLU	2.3
1	A	83	ARG	2.3
1	B	175	GLY	2.2
1	B	185	VAL	2.2
1	A	197	LYS	2.1
1	A	177	SER	2.1
1	A	187	GLU	2.1

## 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	303	4/4	0.71	0.74	72,76,77,77	0
4	EDO	A	302	4/4	0.80	0.38	86,93,93,93	0
5	PEG	A	303	7/7	0.84	0.22	73,73,77,80	0
4	EDO	C	101	4/4	0.85	0.38	70,71,76,77	0
4	EDO	B	301	4/4	0.85	0.17	71,72,80,85	0
4	EDO	A	301	4/4	0.88	0.22	57,62,63,69	0
4	EDO	B	302	4/4	0.89	0.44	75,77,78,79	0
5	PEG	B	305	7/7	0.91	0.30	56,62,70,70	0
5	PEG	B	304	7/7	0.93	0.24	64,69,72,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.