Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 02:13 PM EDT

PDB ID	:	2FIL / pdb_00002fil
Title	:	Crystal Structure Analysis of the A-DNA Decamer GCGT-2'OMeA-faT-AC GC, with Incorporated 2'-O-Methylated-Adenosine (2'OMeA) and 2'-Fluoroa rabino-Thymidine (faT)
Authors	:	Egli, M.; Li, F.
Deposited on	:	2005-12-29
Resolution	:	1.69 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:

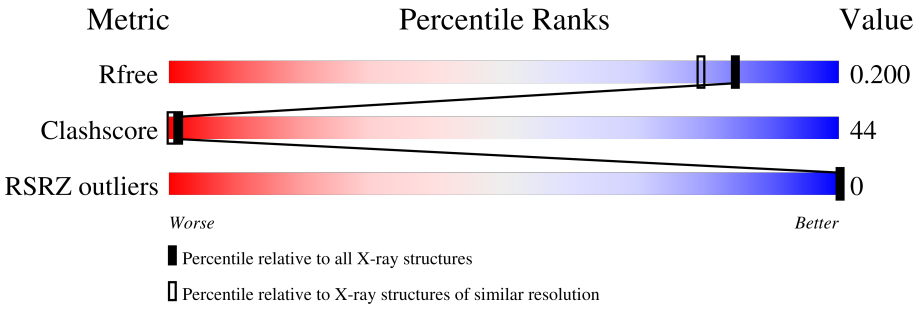
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	10	20% 50% 30%
1	B	10	40% 30% 30%
1	C	10	40% 60%
1	D	10	10% 30% 60%

2 Entry composition (i)

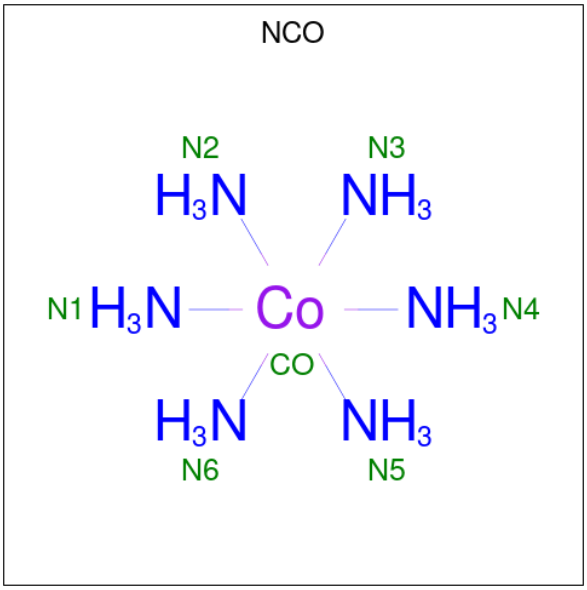
There are 3 unique types of molecules in this entry. The entry contains 1037 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA chain called 5'-D(*GP*CP*GP*TP*(A2M)P*(TAF)P*AP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	10	Total	C	F	N	O	P	0	0	0
			205	98	1	38	59	9			
1	B	10	Total	C	F	N	O	P	0	0	0
			205	98	1	38	59	9			
1	C	10	Total	C	F	N	O	P	0	0	0
			205	98	1	38	59	9			
1	D	10	Total	C	F	N	O	P	0	0	0
			204	98	1	38	58	9			

- Molecule 2 is COBALT HEXAMMINE(III) (CCD ID: NCO) (formula: $CoH_{18}N_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Co	N		0	0
			7	1	6			
2	A	1	Total	Co	N		0	0
			7	1	6			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Co N 7 1 6	0	0
2	B	1	Total Co N 7 1 6	0	0
2	C	1	Total Co N 7 1 6	0	0
2	D	1	Total Co N 7 1 6	0	0
2	D	1	Total Co N 7 1 6	0	0

- Molecule 3 is water.

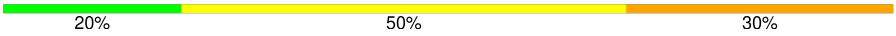
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	48	Total O 48 48	0	0
3	B	31	Total O 31 31	0	0
3	C	42	Total O 42 42	0	0
3	D	48	Total O 48 48	0	0

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: 5'-D(*GP*CP*GP*TP*(A2M)P*(TAF)P*AP*CP*GP*C)-3'

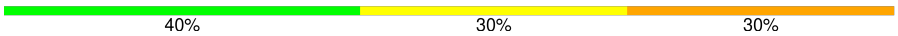
Chain A:





• Molecule 1: 5'-D(*GP*CP*GP*TP*(A2M)P*(TAF)P*AP*CP*GP*C)-3'

Chain B:





• Molecule 1: 5'-D(*GP*CP*GP*TP*(A2M)P*(TAF)P*AP*CP*GP*C)-3'

Chain C:





• Molecule 1: 5'-D(*GP*CP*GP*TP*(A2M)P*(TAF)P*AP*CP*GP*C)-3'

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	32.73Å 69.18Å 32.83Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	30.00 – 1.69 30.00 – 1.69	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.00-1.69) 86.2 (30.00-1.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.215 0.208 , 0.200	Depositor DCC
R_{free} test set	957 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 107.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.247 for l,k,-h 0.287 for h,-k,-l 0.377 for l,-k,h	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	1037	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.28% 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: TAF, NCO, A2M

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	0.66	0/179	1.30	1/272 (0.4%)
1	B	0.68	0/179	1.63	4/272 (1.5%)
1	C	0.60	0/179	1.41	0/272
1	D	0.87	0/178	1.78	7/270 (2.6%)
All	All	0.71	0/715	1.54	12/1086 (1.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	203	DG	O4'-C1'-N9	-7.37	97.35	108.40
1	B	203	DG	C4-N9-C1'	-7.25	116.12	127.00
1	B	203	DG	C8-N9-C1'	7.13	137.70	127.00
1	D	404	DT	C6-C5-C7	-6.87	113.69	124.00
1	D	404	DT	C4-C5-C7	6.04	131.47	122.40
1	A	109	DG	P-O5'-C5'	-5.79	111.31	120.00
1	D	402	DC	C5-C4-N4	-5.49	112.07	120.30
1	B	210	DC	O5'-C5'-C4'	-5.47	102.59	110.80
1	D	402	DC	O5'-C5'-C4'	-5.28	102.88	110.80
1	D	409	DG	N9-C1'-C2'	5.26	121.39	113.50
1	D	402	DC	N3-C4-N4	5.10	125.55	117.90
1	D	408	DC	C6-N1-C1'	5.07	127.31	119.70

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	205	0	114	16	0
1	B	205	0	115	14	0
1	C	205	0	115	9	0
1	D	204	0	115	11	0
2	A	14	0	0	0	0
2	B	14	0	0	1	0
2	C	7	0	0	2	0
2	D	14	0	0	2	0
3	A	48	0	0	5	0
3	B	31	0	0	10	0
3	C	42	0	0	7	0
3	D	48	0	0	2	0
All	All	1037	0	459	50	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 44.

All (50) 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:203:DG:H4'	3:B:1143:HOH:O	1.60	1.01
1:B:206:TAF:H1'	3:B:1150:HOH:O	1.67	0.93
1:B:206:TAF:H3'	3:B:1197:HOH:O	1.70	0.91
1:A:109:DG:H1'	3:A:1147:HOH:O	1.76	0.85
1:A:105:A2M:H5"	1:A:105:A2M:H8	1.69	0.75
1:B:205:A2M:P	3:B:1297:HOH:O	2.44	0.74
1:B:206:TAF:C1'	3:B:1150:HOH:O	2.29	0.72
2:D:3215:NCO:N4	3:D:1159:HOH:O	2.22	0.72
1:B:205:A2M:N7	3:B:1133:HOH:O	2.22	0.71
1:C:303:DG:N3	3:C:1112:HOH:O	2.23	0.71
2:C:3214:NCO:N1	3:C:1089:HOH:O	2.23	0.70
2:C:3214:NCO:N6	3:C:1113:HOH:O	2.26	0.69
1:A:109:DG:N3	3:A:1147:HOH:O	2.26	0.68
1:D:402:DC:OP1	2:D:3216:NCO:N3	2.26	0.68
2:B:3211:NCO:N4	3:B:1072:HOH:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:DT:H2"	1:C:301:DG:C5	2.31	0.66
1:C:310:DC:P	3:C:1126:HOH:O	2.54	0.65
1:A:109:DG:H2'	1:A:110:DC:C6	2.34	0.62
1:A:109:DG:C1'	3:A:1157:HOH:O	2.50	0.59
1:B:208:DC:H5"	1:B:208:DC:H6	1.68	0.58
1:C:307:DA:H2'	1:C:307:DA:OP2	2.05	0.57
1:D:405:A2M:HM'2	1:D:406:TAF:O4'	2.04	0.56
1:A:104:DT:H2"	1:C:301:DG:N7	2.22	0.55
1:B:206:TAF:H4'	3:B:1117:HOH:O	2.05	0.55
1:D:402:DC:C2'	1:D:403:DG:O5'	2.56	0.54
1:A:109:DG:H1'	3:A:1157:HOH:O	2.07	0.53
1:C:303:DG:N2	3:C:1112:HOH:O	2.37	0.52
1:B:205:A2M:H1'	3:B:1167:HOH:O	2.11	0.51
1:D:409:DG:H2'	1:D:410:DC:O4'	2.11	0.50
1:A:105:A2M:H2	1:B:206:TAF:O2	2.12	0.50
1:A:103:DG:H2'	1:A:104:DT:C6	2.48	0.49
1:D:408:DC:H2"	1:D:409:DG:O5'	2.12	0.49
1:B:205:A2M:C1'	3:B:1167:HOH:O	2.60	0.49
1:D:402:DC:H2'	1:D:403:DG:O5'	2.12	0.48
1:A:106:TAF:H2'	1:A:107:DA:H5'	1.96	0.47
1:D:409:DG:N7	3:D:1090:HOH:O	2.35	0.47
1:C:303:DG:C2	3:C:1112:HOH:O	2.65	0.47
1:A:106:TAF:F2'	1:A:107:DA:C8	2.58	0.46
1:A:106:TAF:H6	1:A:106:TAF:O5'	2.15	0.45
1:D:404:DT:OP2	1:D:404:DT:H73	2.16	0.45
1:A:108:DC:P	3:A:1235:HOH:O	2.74	0.45
1:D:407:DA:H2"	1:D:408:DC:O5'	2.15	0.45
1:B:206:TAF:H6	1:B:206:TAF:O5'	2.17	0.45
1:A:109:DG:C2'	1:A:110:DC:O5'	2.66	0.44
1:C:310:DC:H1'	3:C:1171:HOH:O	2.17	0.44
1:B:203:DG:H2'	1:B:204:DT:C6	2.53	0.44
1:D:408:DC:C2'	1:D:409:DG:O5'	2.68	0.41
1:A:104:DT:H1'	1:C:301:DG:C8	2.56	0.41
1:B:205:A2M:H1'	1:B:205:A2M:HM'3	1.92	0.40
1:D:403:DG:H2'	1:D:404:DT:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TAF	B	206	1	19,22,23	0.65	0	27,32,35	1.25	3 (11%)
1	A2M	A	105	1	22,25,26	0.65	0	30,36,39	1.47	3 (10%)
1	A2M	B	205	1	22,25,26	0.65	0	30,36,39	1.09	1 (3%)
1	TAF	D	406	1	19,22,23	0.70	0	27,32,35	0.95	1 (3%)
1	A2M	D	405	1	22,25,26	0.91	0	30,36,39	1.61	5 (16%)
1	A2M	C	305	1	22,25,26	0.46	0	30,36,39	1.11	2 (6%)
1	TAF	A	106	1	19,22,23	0.80	0	27,32,35	1.32	5 (18%)
1	TAF	C	306	1	19,22,23	0.90	1 (5%)	27,32,35	1.96	8 (29%)

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
1	TAF	B	206	1	-	0/7/25/26	0/2/2/2
1	A2M	A	105	1	-	2/9/27/28	0/3/3/3
1	A2M	B	205	1	-	2/9/27/28	0/3/3/3
1	TAF	D	406	1	-	0/7/25/26	0/2/2/2
1	A2M	D	405	1	-	2/9/27/28	0/3/3/3
1	A2M	C	305	1	-	0/9/27/28	0/3/3/3
1	TAF	A	106	1	-	0/7/25/26	0/2/2/2
1	TAF	C	306	1	-	1/7/25/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	306	TAF	F2'-C2'	-2.18	1.36	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	306	TAF	C2'-C3'-C4'	-5.93	94.61	102.43
1	D	405	A2M	O2'-C2'-C1'	5.00	118.49	108.99
1	A	105	A2M	O3'-C3'-C4'	5.00	125.44	111.08
1	C	306	TAF	C5M-C5-C4	4.27	123.34	118.78
1	A	105	A2M	C2'-C3'-C4'	4.10	110.80	101.99
1	B	205	A2M	O2'-C2'-C1'	3.29	115.23	108.99
1	A	106	TAF	C2'-C3'-C4'	-3.20	98.22	102.43
1	A	105	A2M	O3'-C3'-C2'	3.18	120.08	111.19
1	C	306	TAF	C5M-C5-C6	-3.08	118.68	122.85
1	C	306	TAF	C1'-N1-C6	-2.91	116.36	121.15
1	C	305	A2M	O2'-C2'-C1'	2.87	114.44	108.99
1	B	206	TAF	O4-C4-C5	-2.86	121.64	124.92
1	B	206	TAF	C5M-C5-C4	2.73	121.70	118.78
1	A	106	TAF	C5M-C5-C4	2.70	121.66	118.78
1	D	405	A2M	C4-C5-N7	2.53	113.48	110.58
1	D	406	TAF	O4-C4-C5	-2.50	122.06	124.92
1	C	305	A2M	CM'-O2'-C2'	-2.49	108.07	114.47
1	A	106	TAF	O3'-C3'-C2'	2.47	120.94	111.85
1	D	405	A2M	O3'-C3'-C4'	-2.46	104.03	111.08
1	D	405	A2M	C5-C4-N3	2.43	130.06	126.72
1	C	306	TAF	C1'-N1-C2	2.36	121.84	117.59
1	C	306	TAF	C5'-C4'-C3'	2.35	123.69	115.21
1	D	405	A2M	C6-C5-C4	-2.18	114.20	117.18
1	C	306	TAF	C4'-O4'-C1'	-2.14	104.75	109.47
1	B	206	TAF	F2'-C2'-C1'	2.13	113.16	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	306	TAF	O4-C4-C5	-2.09	122.53	124.92
1	A	106	TAF	O2-C2-N1	2.07	125.48	122.80
1	A	106	TAF	C5M-C5-C6	-2.01	120.13	122.85

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	105	A2M	C3'-C4'-C5'-O5'
1	D	405	A2M	O4'-C4'-C5'-O5'
1	A	105	A2M	O4'-C4'-C5'-O5'
1	B	205	A2M	O4'-C4'-C5'-O5'
1	C	306	TAF	C4'-C5'-O5'-P
1	D	405	A2M	C3'-C4'-C5'-O5'
1	B	205	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	206	TAF	6	0
1	A	105	A2M	2	0
1	B	205	A2M	5	0
1	D	406	TAF	1	0
1	D	405	A2M	1	0
1	A	106	TAF	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
2	NCO	D	3215	-	6,6,6	0.56	0	-		
2	NCO	D	3216	-	6,6,6	0.68	0	-		
2	NCO	A	3212	-	6,6,6	0.69	0	-		
2	NCO	C	3214	-	6,6,6	0.69	0	-		
2	NCO	B	3217	-	6,6,6	0.57	0	-		
2	NCO	A	3213	-	6,6,6	0.54	0	-		
2	NCO	B	3211	-	6,6,6	0.77	0	-		

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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3215	NCO	1	0
2	D	3216	NCO	1	0
2	C	3214	NCO	2	0
2	B	3211	NCO	1	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	8/10 (80%)	-0.85	0	100	100	40, 42, 53, 60	0
1	B	8/10 (80%)	-0.68	0	100	100	36, 43, 57, 66	0
1	C	8/10 (80%)	-0.86	0	100	100	36, 44, 50, 53	0
1	D	8/10 (80%)	-0.73	0	100	100	35, 40, 50, 51	0
All	All	32/40 (80%)	-0.78	0	100	100	35, 43, 57, 66	0

There are no RSRZ outliers to report.

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

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
1	TAF	A	106	21/22	0.98	0.06	44,57,68,73	0
1	A2M	B	205	23/24	0.98	0.06	38,44,50,51	0
1	TAF	B	206	21/22	0.98	0.06	48,56,62,66	0
1	A2M	D	405	23/24	0.98	0.05	25,36,47,56	0
1	A2M	C	305	23/24	0.99	0.06	36,46,52,60	0
1	TAF	C	306	21/22	0.99	0.05	42,53,59,64	0
1	A2M	A	105	23/24	0.99	0.06	46,50,60,63	0
1	TAF	D	406	21/22	0.99	0.06	40,47,53,58	0

6.3 Carbohydrates

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, 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
2	NCO	B	3217	7/7	0.98	0.08	135,135,136,136	0
2	NCO	D	3216	7/7	0.98	0.06	67,69,73,74	0
2	NCO	B	3211	7/7	0.99	0.05	54,60,65,67	0
2	NCO	A	3212	7/7	0.99	0.06	56,62,64,65	0
2	NCO	C	3214	7/7	0.99	0.05	42,53,56,56	0
2	NCO	D	3215	7/7	0.99	0.06	20,24,26,28	0
2	NCO	A	3213	7/7	0.99	0.05	68,72,76,78	0

6.5 Other polymers (i)

There are no such residues in this entry.