wwPDB X-ray Structure Validation Summary Report (i)

Nov 13, 2023 – 10:31 PM JST

PDB ID	:	5Y7G
Title	:	Crystal structure of paFAN1 bound to 1nt 5'flap DNA with gap
Authors	:	Cho, Y.; Jin, H.
Deposited on	:	2017-08-17
Resolution	:	3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

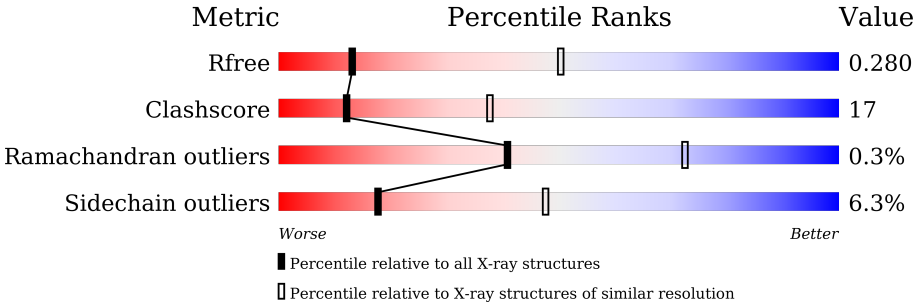
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)

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%

Mol	Chain	Length	Quality of chain
1	A	580	59% 30% • 7%
1	B	580	60% 31% • 6%
1	C	580	61% 30% • 7%
2	D	10	20% 50% 30%
2	F	10	40% 50% 10%
2	H	10	10% 90%
3	E	24	25% 50% 25%

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Mol	Chain	Length	Quality of chain
3	G	24	38% 54% 8%
3	I	24	29% 71%
4	J	14	29% 43% 29%
4	L	14	14% 71% 14%
4	N	14	7% 86% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16164 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 Fanconi-associated nuclease 1 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	542	4406	2816	799	771	20	0	0	0
1	B	543	4424	2827	800	777	20	0	0	0
1	C	540	4401	2813	794	774	20	0	0	0

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q9I2N0
A	-19	GLY	-	expression tag	UNP Q9I2N0
A	-18	SER	-	expression tag	UNP Q9I2N0
A	-17	SER	-	expression tag	UNP Q9I2N0
A	-16	HIS	-	expression tag	UNP Q9I2N0
A	-15	HIS	-	expression tag	UNP Q9I2N0
A	-14	HIS	-	expression tag	UNP Q9I2N0
A	-13	HIS	-	expression tag	UNP Q9I2N0
A	-12	HIS	-	expression tag	UNP Q9I2N0
A	-11	HIS	-	expression tag	UNP Q9I2N0
A	-10	SER	-	expression tag	UNP Q9I2N0
A	-9	SER	-	expression tag	UNP Q9I2N0
A	-8	GLY	-	expression tag	UNP Q9I2N0
A	-7	LEU	-	expression tag	UNP Q9I2N0
A	-6	VAL	-	expression tag	UNP Q9I2N0
A	-5	PRO	-	expression tag	UNP Q9I2N0
A	-4	ARG	-	expression tag	UNP Q9I2N0
A	-3	GLY	-	expression tag	UNP Q9I2N0
A	-2	SER	-	expression tag	UNP Q9I2N0
A	-1	HIS	-	expression tag	UNP Q9I2N0
A	0	MET	-	expression tag	UNP Q9I2N0
B	-20	MET	-	expression tag	UNP Q9I2N0
B	-19	GLY	-	expression tag	UNP Q9I2N0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	SER	-	expression tag	UNP Q9I2N0
B	-17	SER	-	expression tag	UNP Q9I2N0
B	-16	HIS	-	expression tag	UNP Q9I2N0
B	-15	HIS	-	expression tag	UNP Q9I2N0
B	-14	HIS	-	expression tag	UNP Q9I2N0
B	-13	HIS	-	expression tag	UNP Q9I2N0
B	-12	HIS	-	expression tag	UNP Q9I2N0
B	-11	HIS	-	expression tag	UNP Q9I2N0
B	-10	SER	-	expression tag	UNP Q9I2N0
B	-9	SER	-	expression tag	UNP Q9I2N0
B	-8	GLY	-	expression tag	UNP Q9I2N0
B	-7	LEU	-	expression tag	UNP Q9I2N0
B	-6	VAL	-	expression tag	UNP Q9I2N0
B	-5	PRO	-	expression tag	UNP Q9I2N0
B	-4	ARG	-	expression tag	UNP Q9I2N0
B	-3	GLY	-	expression tag	UNP Q9I2N0
B	-2	SER	-	expression tag	UNP Q9I2N0
B	-1	HIS	-	expression tag	UNP Q9I2N0
B	0	MET	-	expression tag	UNP Q9I2N0
C	-20	MET	-	expression tag	UNP Q9I2N0
C	-19	GLY	-	expression tag	UNP Q9I2N0
C	-18	SER	-	expression tag	UNP Q9I2N0
C	-17	SER	-	expression tag	UNP Q9I2N0
C	-16	HIS	-	expression tag	UNP Q9I2N0
C	-15	HIS	-	expression tag	UNP Q9I2N0
C	-14	HIS	-	expression tag	UNP Q9I2N0
C	-13	HIS	-	expression tag	UNP Q9I2N0
C	-12	HIS	-	expression tag	UNP Q9I2N0
C	-11	HIS	-	expression tag	UNP Q9I2N0
C	-10	SER	-	expression tag	UNP Q9I2N0
C	-9	SER	-	expression tag	UNP Q9I2N0
C	-8	GLY	-	expression tag	UNP Q9I2N0
C	-7	LEU	-	expression tag	UNP Q9I2N0
C	-6	VAL	-	expression tag	UNP Q9I2N0
C	-5	PRO	-	expression tag	UNP Q9I2N0
C	-4	ARG	-	expression tag	UNP Q9I2N0
C	-3	GLY	-	expression tag	UNP Q9I2N0
C	-2	SER	-	expression tag	UNP Q9I2N0
C	-1	HIS	-	expression tag	UNP Q9I2N0
C	0	MET	-	expression tag	UNP Q9I2N0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	10	211	100	38	63	10	0	0	0
2	F	10	211	100	38	63	10	0	0	0
2	H	10	211	100	38	63	10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	24	488	234	84	146	24	0	0	0
3	G	24	487	233	84	146	24	0	0	0
3	I	24	488	234	84	146	24	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(P*TP*GP*AP*CP*AP*CP*AP*CP*AP*TP*TP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	J	14	284	136	53	81	14	0	0	0
4	L	14	284	136	53	81	14	0	0	0
4	N	13	264	126	51	74	13	0	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

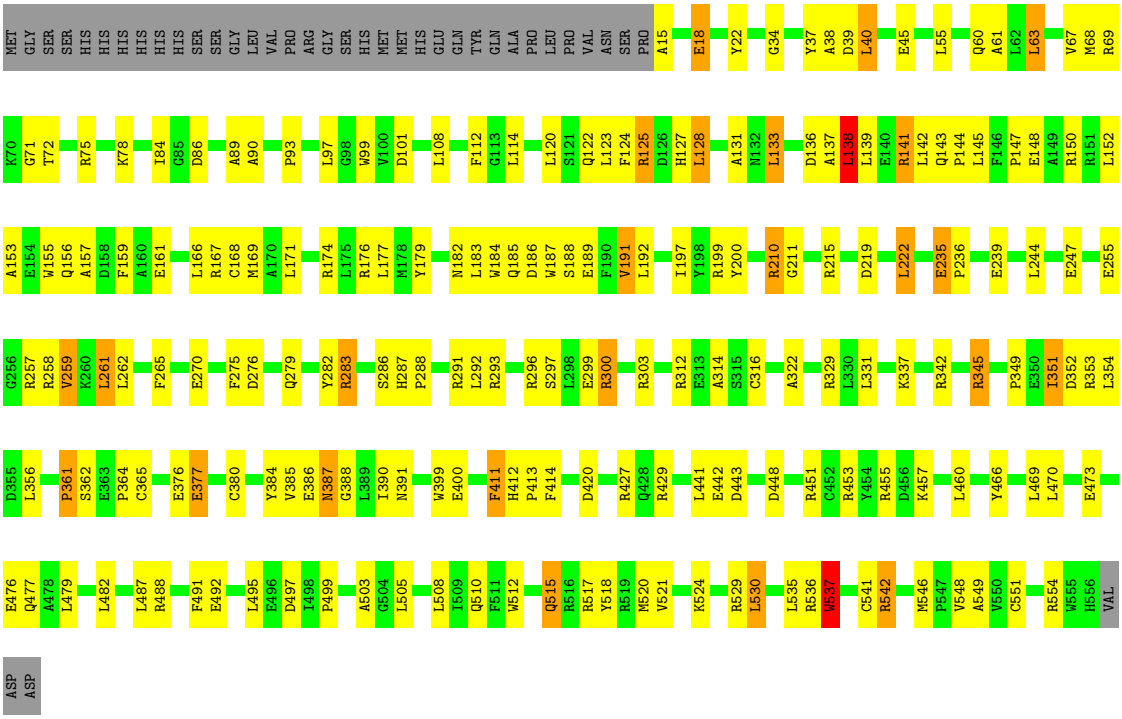
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	2	2	2	0	0
5	B	2	2	2	0	0
5	C	1	1	1	0	0

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

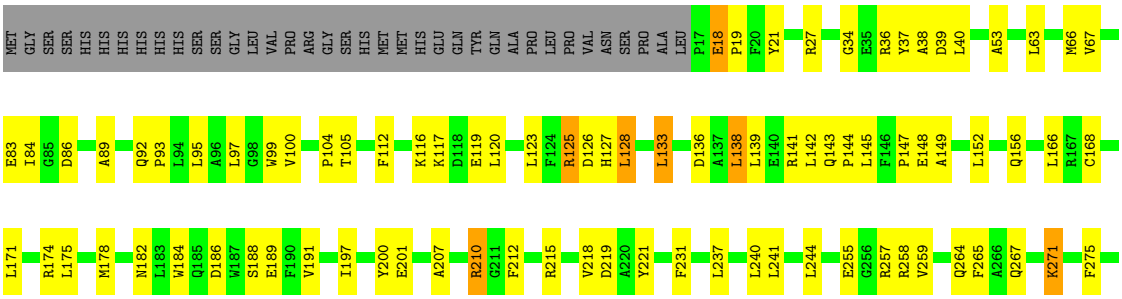
- Molecule 1: Fanconi-associated nuclease 1 homolog

Chain A:



- Molecule 1: Fanconi-associated nuclease 1 homolog

Chain B:



Q279 R280 L281 Y282 R283 H287 P288 G289 L292 R293 A294 I295 R296 S297 L298 E299 R300 G301 E302 R303 F304 L310 A311 A314 E323 L327 L331 P332 R333 L334 L338 Q343 A344 R345 E350 I351 D352 R353 L354 D355 L356 F360 P361 S362 E363 P364 C365 S366 V367

E368 W369 C380 A381 Y384 V385 E386 N387 G388 L389 I390 L393 F394 W399 E400 I406 F411 H412 P413 F414 A417 D420 L421 H422 S423 R430 L433 L441 E442 R447 R451 C452 R453 Y454 R455 F458 G459 L460 P463 F464 V465 Y466 W467 E468 L469

E473 L474 Q477 R488 A489 W490 F491 L494 D497 I498 P499 G500 N501 R502 L505 P506 D507 L508 I509 Q510 F511 W512 Q515 R516 R517 Y518 E522 V523 K524 L530 L535 R536 W537 F540 C541 R542 E543 R544 P547 C551 Y552 D558 D559

- Molecule 1: Fanconi-associated nuclease 1 homolog

Chain C: 61% 30% • 7%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET MET HIS GLU GLN TYR GLN ALA PRO LEU PRO VAL ASN SER PRO ALA LEU PRO E18 P19 F20 Y21 L30 A31 W32 I33 G34 E35 R36 Y37 A38 D39 L40 L41 Q44 E45 F48

I49 F52 L55 Q60 A61 L62 R69 K70 G71 T72 L73 F74 R75 E76 E83 I84 G85 D86 T87 R88 A89 A90 V91 L95 W99 V100 P104 T105 L106 E107 L108 K116 E119 R125 L128 R134 K135 D136 A137 L138 L139 E140 R141 L142 F146 P147

R151 E154 D158 F159 A160 E161 Y164 E165 R174 L175 Y179 F180 G181 N182 L183 W184 Q185 E189 L192 Y200 S209 R210 G211 F212 R213 P236 L237 E238 E239 L244 P245 Y249 W253 F265 K271 D276 R283 S286 H287 P288

R291 T295 R296 E299 R300 R303 L310 A311 R312 E313 E319 E323 L327 L330 L331 P332 R333 L334 Q335 Q343 A344 R345 A346 A347 A348 P349 E350 I351 D352 R353 L354 D355 L356 C357 L358 A359 F360 P361 S362 E363 P364 C365 E368 R372 E376 Y384 V385

E386 N387 G388 L389 I390 F394 W399 F411 H412 P413 F414 D420 L421 H422 R430 F434 C437 R440 L441 E442 R447 R451 C452 R453 Y454 R455 D456 K457 F458 G459 L460 E468 L469 E473 E476 Q477 A478 L479 L487 R488 F491 L495 E496 D497

I498 P499 G500 N501 L505 P506 Q515 ARG R517 M520 V523 K524 L530 N533 Q534 L535 R536 W537 L538 Q539 F540 C541 R542 E543 R544 V548 C551 H556 V557 D558 ASP

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

Chain D: 20% 50% 30%

G1 T2 T3 G4 G5 G6 A7 T8 T9 G10

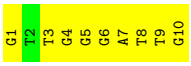
- Molecule 2: DNA (5'-D(P*GP*TP*TP*GP*GP*GP*AP*TP*TP*G)-3')

Chain F: 40% 50% 10%

G1 T2 G5 G6 A7 G10

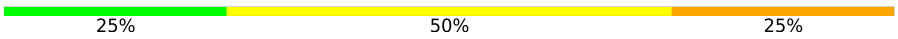
- Molecule 2: DNA (5'-D(P*GP*TP*TP*GP*GP*GP*AP*TP*TP*G)-3')

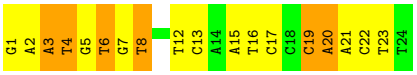
Chain H: 10% 90%



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

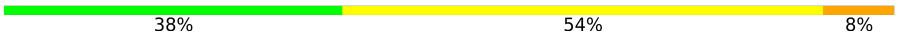
Chain E:





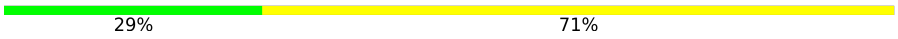
• Molecule 3: DNA (5'-D(P*GP*AP*AP*TP*GP*TP*GP*TP*GP*TP*CP*TP*CP*AP*AP*TP*CP*CP*CP*AP*AP*CP*TP*T)-3')

Chain G:



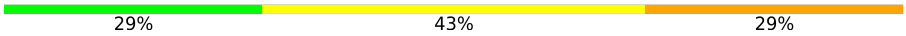
• Molecule 3: DNA (5'-D(P*GP*AP*AP*TP*GP*TP*GP*TP*GP*TP*CP*TP*CP*AP*AP*TP*CP*CP*CP*AP*AP*CP*TP*T)-3')

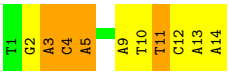
Chain I:



• Molecule 4: DNA (5'-D(P*TP*GP*AP*CP*AP*CP*AP*CP*AP*TP*TP*CP*AP*A)-3')

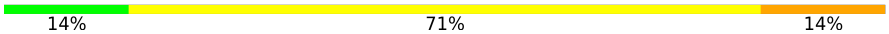
Chain J:

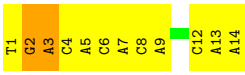




• Molecule 4: DNA (5'-D(P*TP*GP*AP*CP*AP*CP*AP*CP*AP*TP*TP*CP*AP*A)-3')

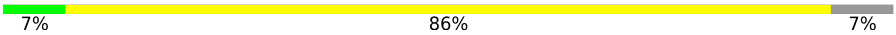
Chain L:

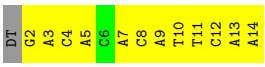




• Molecule 4: DNA (5'-D(P*TP*GP*AP*CP*AP*CP*AP*CP*AP*TP*TP*CP*AP*A)-3')

Chain N:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	140.29Å 143.26Å 172.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.58 – 3.40 46.03 – 3.17	Depositor EDS
% Data completeness (in resolution range)	95.6 (33.58-3.40) 94.4 (46.03-3.17)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.10.1-2155_1069: ???)	Depositor
R, R_{free}	0.221 , 0.280 0.221 , 0.280	Depositor DCC
R_{free} test set	2841 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	105.5	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 64.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.004 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16164	wwPDB-VP
Average B, all atoms (Å^2)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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 (i)

5.1 Standard geometry (i)

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

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	0.62	1/4522 (0.0%)	0.87	7/6125 (0.1%)
1	B	0.55	1/4541 (0.0%)	0.79	4/6150 (0.1%)
1	C	0.47	0/4516	0.72	1/6115 (0.0%)
2	D	1.26	2/236 (0.8%)	1.25	2/364 (0.5%)
2	F	1.09	1/236 (0.4%)	1.10	0/364
2	H	0.76	0/236	1.11	0/364
3	E	1.43	6/545 (1.1%)	1.18	5/838 (0.6%)
3	G	1.17	3/544 (0.6%)	1.15	1/836 (0.1%)
3	I	1.00	0/545	1.12	0/838
4	J	1.42	3/318 (0.9%)	1.17	2/487 (0.4%)
4	L	1.08	1/318 (0.3%)	1.05	1/487 (0.2%)
4	N	0.82	0/296	0.94	0/453
All	All	0.71	18/16853 (0.1%)	0.88	23/23421 (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
1	A	0	2
1	B	0	1
All	All	0	3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	12	DT	C1'-N1	8.56	1.60	1.49
3	E	4	DT	C3'-O3'	-8.22	1.33	1.44
2	F	7	DA	C3'-O3'	-7.67	1.33	1.44
2	D	7	DA	C3'-O3'	-7.26	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	4	DC	C3'-O3'	-6.70	1.35	1.44

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	7	DA	O5'-P-OP2	-8.03	98.47	105.70
4	J	3	DA	O5'-P-OP2	-7.43	99.01	105.70
1	A	377	GLU	C-N-CD	-7.32	104.49	120.60
4	L	2	DG	O4'-C4'-C3'	-6.84	101.76	104.50
3	E	4	DT	O4'-C4'-C3'	-6.81	101.78	104.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	PRO	Peptide
1	A	71	GLY	Peptide
1	B	361	PRO	Peptide

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	4406	0	4306	149	1
1	B	4424	0	4317	139	0
1	C	4401	0	4293	129	1
2	D	211	0	115	16	0
2	F	211	0	115	5	0
2	H	211	0	115	14	0
3	E	488	0	273	16	0
3	G	487	0	270	15	0
3	I	488	0	273	20	0
4	J	284	0	158	11	0
4	L	284	0	158	16	0
4	N	264	0	146	11	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
All	All	16164	0	14539	524	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 524 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:342:ARG:NH1	4:J:14:DA:OP1	1.91	1.03
1:B:387:ASN:HB3	1:B:505:LEU:HB2	1.48	0.96
3:E:21:DA:H2"	3:E:22:DC:H5"	1.49	0.94
3:G:21:DA:H2"	3:G:22:DC:H5"	1.49	0.94
4:N:9:DA:H2"	4:N:10:DT:H5"	1.50	0.93

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLU:O	1:C:447:ARG:NH2[3_545]	2.18	0.02

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	540/580 (93%)	520 (96%)	18 (3%)	2 (0%)	34	67
1	B	541/580 (93%)	523 (97%)	16 (3%)	2 (0%)	34	67
1	C	536/580 (92%)	511 (95%)	24 (4%)	1 (0%)	47	78
All	All	1617/1740 (93%)	1554 (96%)	58 (4%)	5 (0%)	41	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	361	PRO
1	A	18	GLU
1	B	344	ALA
1	B	19	PRO
1	A	235	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	441/478 (92%)	406 (92%)	35 (8%)	12	39
1	B	444/478 (93%)	422 (95%)	22 (5%)	24	54
1	C	442/478 (92%)	416 (94%)	26 (6%)	19	49
All	All	1327/1434 (92%)	1244 (94%)	83 (6%)	18	47

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	18	GLU
1	C	327	LEU
1	C	60	GLN
1	C	174	ARG
1	C	411	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	279	GLN
1	C	343	GLN
1	C	531	GLN
1	C	533	ASN

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 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.