wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 04:56 PM GMT

PDB ID	:	4GFH
Title	:	Topoisomerase II-DNA-AMPPNP complex
Authors	:	Schmidt, B.H.; Osheroff, N.; Berger, J.M.
Deposited on	:	2012-08-03
Resolution	:	4.41 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

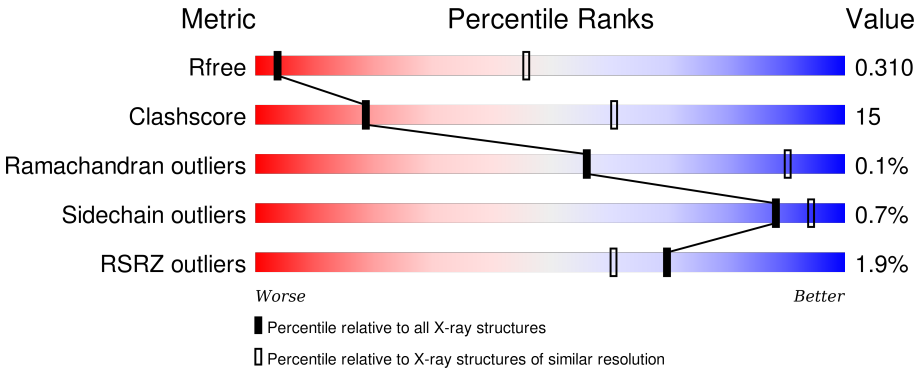
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 4.41 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}	91344	1067 (5.20-3.60)
Clashscore	102246	1175 (5.20-3.60)
Ramachandran outliers	100387	1114 (5.20-3.60)
Sidechain outliers	100360	1096 (5.20-3.60)
RSRZ outliers	91569	1071 (5.20-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	1178	2% 65% 27% • 6%
1	F	1178	% 65% 27% • 7%
2	B	11	27% 64% 9%
2	G	11	45% 45% 9%
3	C	15	47% 53%

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Mol	Chain	Length	Quality of chain
3	H	15	47% 53%
4	D	11	91% 9%
4	I	11	73% 18% 9%
5	E	15	73% 27%
5	J	15	60% 40%

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
1	PTR	F	782[A]	-	-	X	-
4	TSP	I	11[B]	-	-	-	X
6	MG	A	1201	-	-	-	X
7	ANP	A	1202	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20236 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 DNA topoisomerase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1102	Total	C	N	O	P	S	0	1	0
			9042	5804	1515	1687	1	35			
1	F	1098	Total	C	N	O	P	S	0	1	0
			9012	5788	1510	1678	1	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	11	0
			219	105	36	67	11			
2	G	11	Total	C	N	O	P	0	11	0
			219	105	36	67	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	P	0	15	0
			310	147	63	86	14			
3	H	15	Total	C	N	O	P	0	15	0
			310	147	63	86	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	S	0	11	0
			230	109	44	65	11	1			
4	I	11	Total	C	N	O	P	S	0	11	0
			230	109	44	65	11	1			

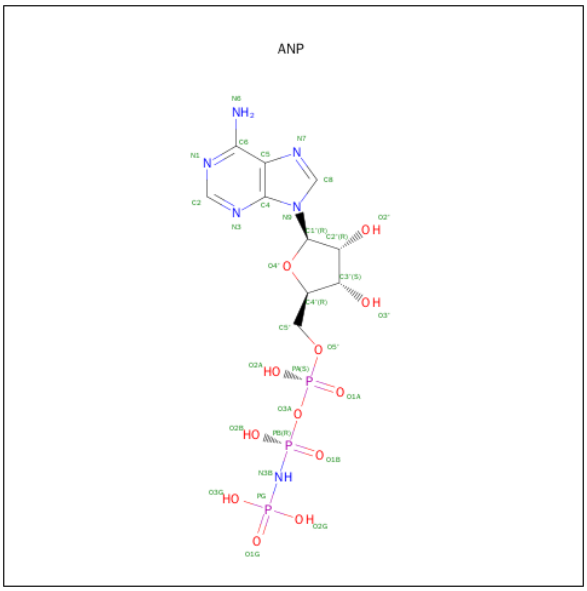
- Molecule 5 is a DNA chain called DNA (5'-D(*CP*GP*CP*GP*AP*AP*TP*CP*GP*TP*CP*AP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	15	Total	C	N	O	P	0	15	0
			300	144	54	88	14			
5	J	15	Total	C	N	O	P	0	15	0
			300	144	54	88	14			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



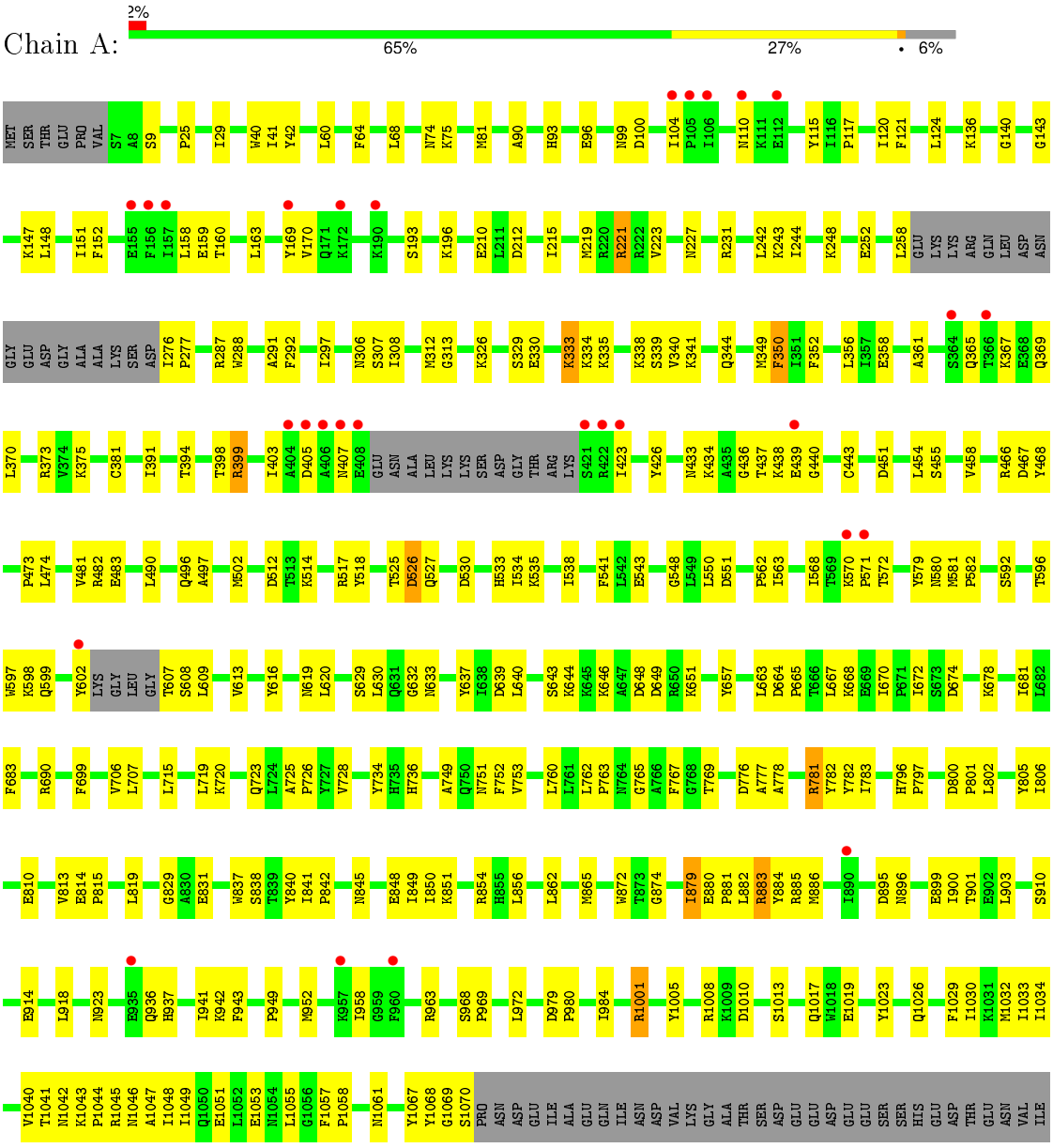
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

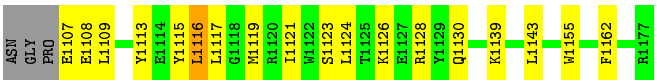
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: DNA topoisomerase 2

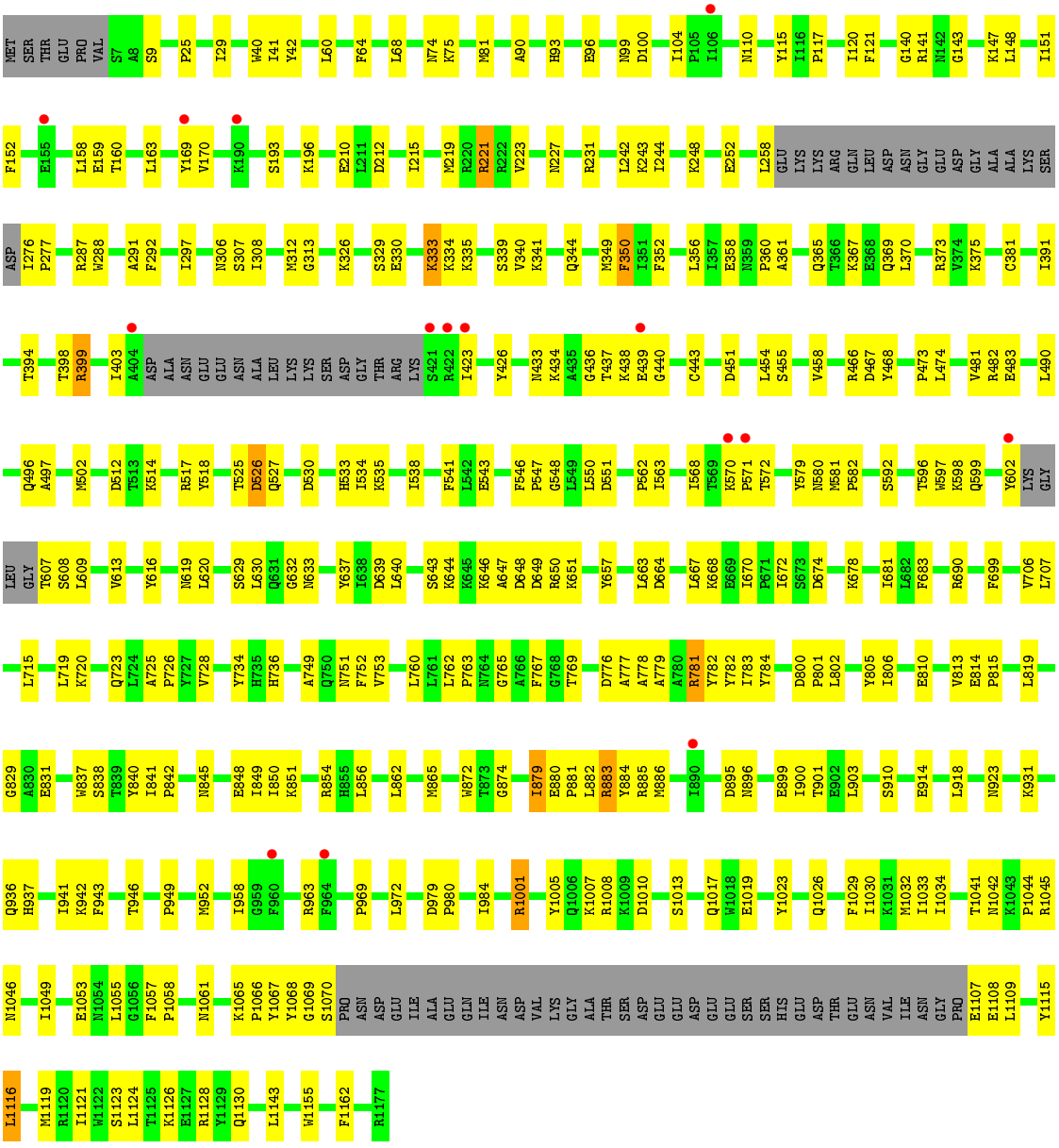
Chain A:





• Molecule 1: DNA topoisomerase 2

Chain F:

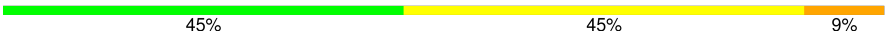


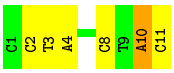
• Molecule 2: DNA (5'-D(P*CP*CP*TP*AP*CP*TP*GP*CP*TP*AP*C)-3')

Chain B:

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

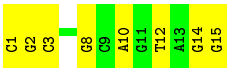
Chain G:





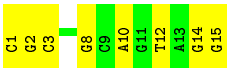
• Molecule 3: DNA (5'-D(*CP*GP*CP*GP*GP*TP*AP*GP*CP*AP*GP*TP*AP*GP*G)-3')

Chain C:



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

Chain H:



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

Chain D:

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

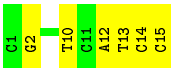
Chain I:

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

Chain E:

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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	169.13Å 169.88Å 169.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.99 – 4.41 46.99 – 4.41	Depositor EDS
% Data completeness (in resolution range)	91.2 (46.99-4.41) 91.0 (46.99-4.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 4.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.239 , 0.275 0.285 , 0.310	Depositor DCC
R_{free} test set	1458 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	185.0	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 184.3	EDS
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -k,-h,-l 0.389 for l,-k,h 0.000 for l,h,k 0.000 for k,l,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 28687 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	20236	wwPDB-VP
Average B, all atoms (Å^2)	248.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ANP, PTR, TSP

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	0.23	0/9218	0.45	2/12428 (0.0%)
1	F	0.23	0/9188	0.45	2/12387 (0.0%)
2	B	0.39	0/243	1.00	1/371 (0.3%)
2	G	0.39	0/243	0.99	1/371 (0.3%)
3	C	0.58	2/349 (0.6%)	0.96	0/539
3	H	0.46	0/349	0.98	0/539
4	D	0.47	0/236	0.94	1/363 (0.3%)
4	I	0.41	0/236	0.97	2/363 (0.6%)
5	E	0.43	0/335	0.98	0/514
5	J	0.43	0/335	0.95	0/514
All	All	0.26	2/20732 (0.0%)	0.54	9/28389 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1[A]	DC	C4'-O4'	5.23	1.50	1.45
3	C	1[A]	DC	O3'-P	-5.03	1.55	1.61

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	10[B]	DT	C4'-C3'-O3'	6.17	125.13	109.70
2	G	10[A]	DA	O4'-C4'-C3'	-5.83	102.17	104.50
2	B	10[A]	DA	O4'-C4'-C3'	-5.75	102.20	104.50
1	A	879	ILE	CB-CA-C	-5.57	100.45	111.60
1	F	879	ILE	CB-CA-C	-5.56	100.48	111.60

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	9042	0	9077	308	0
1	F	9012	0	9056	306	0
2	B	219	0	114	8	0
2	G	219	0	118	7	0
3	C	310	0	146	7	0
3	H	310	0	147	8	0
4	D	230	0	108	1	0
4	I	230	0	108	6	0
5	E	300	0	154	3	0
5	J	300	0	153	7	0
6	A	1	0	0	0	0
6	F	1	0	0	0	0
7	A	31	0	13	2	0
7	F	31	0	13	3	0
All	All	20236	0	19207	609	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 15.

The worst 5 of 609 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:F:29:ILE:HD13	1:F:152:PHE:CE2	1.73	1.24
1:A:29:ILE:HD13	1:A:152:PHE:CE2	1.73	1.23
1:F:29:ILE:CD1	1:F:152:PHE:CZ	2.38	1.06
1:A:29:ILE:CD1	1:A:152:PHE:CZ	2.38	1.05
1:A:29:ILE:HD13	1:A:152:PHE:CZ	1.93	1.02

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	1091/1178 (93%)	1038 (95%)	52 (5%)	1 (0%)	56 90
1	F	1087/1178 (92%)	1034 (95%)	52 (5%)	1 (0%)	56 90
All	All	2178/2356 (92%)	2072 (95%)	104 (5%)	2 (0%)	56 90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	526	ASP
1	F	526	ASP

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	992/1055 (94%)	985 (99%)	7 (1%)	88 94
1	F	989/1055 (94%)	982 (99%)	7 (1%)	88 94
All	All	1981/2110 (94%)	1967 (99%)	14 (1%)	88 94

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1001	ARG
1	F	221	ARG
1	F	781	ARG
1	A	883	ARG

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Mol	Chain	Res	Type
1	F	399	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1167	GLN
1	F	1167	GLN
1	F	227	ASN
1	A	496	GLN
1	F	99	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)

4 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	PTR	A	782[A]	1	14,16,17	1.95	1 (7%)	18,22,24	0.70	0
4	TSP	D	11[B]	4	10,21,22	2.87	4 (40%)	11,30,33	2.44	3 (27%)
1	PTR	F	782[A]	1	14,16,17	1.96	1 (7%)	18,22,24	0.70	0
4	TSP	I	11[B]	4	10,21,22	2.85	4 (40%)	11,30,33	2.45	4 (36%)

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	PTR	A	782[A]	1	-	0/9/11/13	0/1/1/1
4	TSP	D	11[B]	4	-	0/3/21/22	0/2/2/2
1	PTR	F	782[A]	1	-	0/9/11/13	0/1/1/1
4	TSP	I	11[B]	4	-	0/3/21/22	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	782[A]	PTR	OH-CZ	-7.19	1.23	1.40
1	A	782[A]	PTR	OH-CZ	-7.15	1.23	1.40
4	D	11[B]	TSP	O4'-C4'	-3.18	1.37	1.45
4	I	11[B]	TSP	O4'-C4'	-3.13	1.37	1.45
4	I	11[B]	TSP	C6-N1	3.97	1.40	1.35

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	11[B]	TSP	C5-C4-N3	-4.50	120.12	125.14
4	I	11[B]	TSP	C5-C4-N3	-4.38	120.26	125.14
4	D	11[B]	TSP	O4'-C1'-N1	2.05	111.27	107.72
4	I	11[B]	TSP	O4'-C1'-N1	2.11	111.37	107.72
4	I	11[B]	TSP	O5'-C5'-C4'	2.36	117.77	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	782[A]	PTR	1	0
1	F	782[A]	PTR	6	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
7	ANP	A	1202	6	27,33,33	1.72	9 (33%)	30,52,52	1.92	3 (10%)
7	ANP	F	1202	6	27,33,33	1.73	9 (33%)	30,52,52	1.91	3 (10%)

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
7	ANP	A	1202	6	-	0/12/38/38	0/3/3/3
7	ANP	F	1202	6	-	0/12/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	1202	ANP	PG-O3G	-2.38	1.50	1.56
7	A	1202	ANP	PG-O3G	-2.38	1.50	1.56
7	A	1202	ANP	PG-O2G	-2.34	1.50	1.56
7	F	1202	ANP	PG-O2G	-2.34	1.50	1.56
7	F	1202	ANP	O4'-C4'	-2.34	1.39	1.45

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1202	ANP	N3-C2-N1	-7.49	123.16	128.89
7	F	1202	ANP	N3-C2-N1	-7.42	123.21	128.89
7	A	1202	ANP	PA-O3A-PB	-3.26	121.75	132.67
7	F	1202	ANP	PA-O3A-PB	-3.25	121.78	132.67
7	A	1202	ANP	C4'-O4'-C1'	3.64	113.72	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1202	ANP	2	0
7	F	1202	ANP	3	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	1101/1178 (93%)	0.03	29 (2%) 59 49	150, 238, 317, 403	0
1	F	1097/1178 (93%)	0.01	15 (1%) 78 69	146, 240, 314, 414	0
2	B	11/11 (100%)	0.55	0 100 100	174, 267, 347, 364	11 (100%)
2	G	11/11 (100%)	0.59	0 100 100	158, 225, 331, 333	11 (100%)
3	C	15/15 (100%)	0.03	0 100 100	216, 271, 425, 430	15 (100%)
3	H	15/15 (100%)	0.16	0 100 100	203, 265, 377, 431	15 (100%)
4	D	10/11 (90%)	0.44	0 100 100	165, 245, 364, 429	10 (100%)
4	I	10/11 (90%)	0.52	0 100 100	169, 275, 401, 418	10 (100%)
5	E	15/15 (100%)	0.03	0 100 100	162, 253, 360, 382	15 (100%)
5	J	15/15 (100%)	0.18	0 100 100	180, 292, 332, 376	15 (100%)
All	All	2300/2460 (93%)	0.03	44 (1%) 70 61	146, 240, 322, 431	102 (4%)

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	422	ARG	5.2
1	A	406	ALA	4.2
1	F	421	SER	4.2
1	F	570	LYS	3.5
1	A	172	LYS	3.4

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	TSP	I	11[B]	20/21	0.83	0.41	0.72	429,437,440,441	20
4	TSP	D	11[B]	20/21	0.83	0.36	0.27	501,508,514,517	20
1	PTR	F	782[A]	16/17	0.81	0.40	-	299,305,310,312	16
1	PTR	A	782[A]	16/17	0.70	0.51	-	281,285,288,289	16

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
6	MG	A	1201	1/1	0.98	0.42	1.55	115,115,115,115	0
6	MG	F	1201	1/1	0.98	0.39	1.37	114,114,114,114	0
7	ANP	F	1202	31/31	0.87	0.38	0.37	229,235,247,251	0
7	ANP	A	1202	31/31	0.85	0.41	0.31	230,235,236,237	0

6.5 Other polymers (i)

There are no such residues in this entry.