W O R L D W I D E
wwPDB
P R O T E I N D A T A B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2017 – 01:30 am GMT

PDB ID	:	2J0Q
Title	:	THE CRYSTAL STRUCTURE OF THE EXON JUNCTION COMPLEX AT 3.2 A RESOLUTION
Authors	:	Bono, F.; Ebert, J.; Lorentzen, E.; Conti, E.
Deposited on	:	2006-08-04
Resolution	:	3.20 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

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 3.20 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	Percentile Ranks	Value
Rfree		0.282
Clashscore		5
Ramachandran outliers		1.4%
Sidechain outliers		7.0%
RSRZ outliers		3.3%
RNA backbone		0.18

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
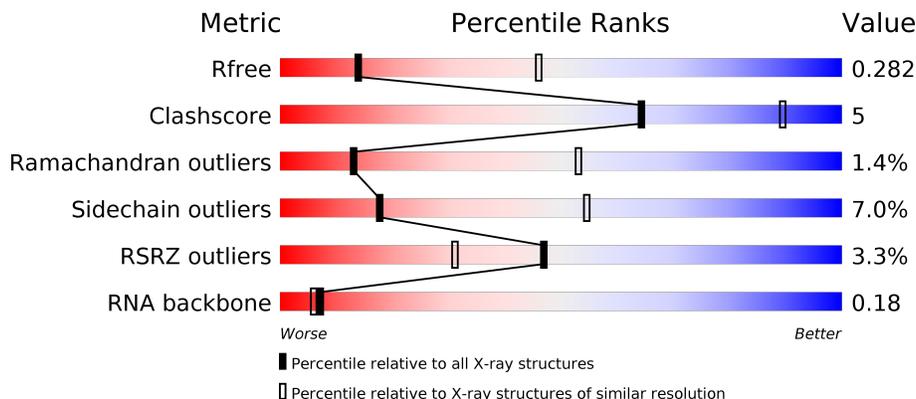
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)
RNA backbone	2435	1045 (3.60-2.80)

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	410	81% 12% • 5%
1	B	410	81% 12% • 5%
2	C	146	86% 12% •
2	F	146	82% 16% •
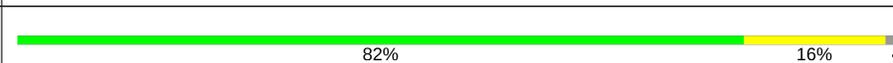
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Mol	Chain	Length	Quality of chain
3	D	109	6% 63% 17% • 18%
3	G	109	6% 68% 14% 18%
4	E	15	7% 33% 60%
4	H	15	20% 7% 13% 60%
5	I	150	8% 29% 13% 58%
5	T	150	8% 33% 8% •• 57%

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
6	MG	B	1412	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11226 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 ATP-DEPENDENT RNA HELICASE DDX48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3073	1944	533	577	19			
1	B	390	Total	C	N	O	S	0	0	0
			3081	1949	535	578	19			

- Molecule 2 is a protein called PROTEIN MAGO NASHI HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	143	Total	C	N	O	S	0	0	0
			1178	764	197	214	3			
2	F	143	Total	C	N	O	S	0	0	0
			1178	764	197	214	3			

- Molecule 3 is a protein called RNA-BINDING PROTEIN 8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	89	Total	C	N	O	S	0	0	0
			688	440	115	130	3			
3	G	89	Total	C	N	O	S	0	0	0
			688	440	115	130	3			

- Molecule 4 is a RNA chain called 5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	6	Total	C	N	O	P	0	0	0
			121	54	12	49	6			
4	H	6	Total	C	N	O	P	0	0	0
			121	54	12	49	6			

- Molecule 5 is a protein called PROTEIN CASC3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	63	Total	C	N	O	0	0	0
			495	306	92	97			
5	T	65	Total	C	N	O	0	0	0
			538	332	102	104			

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

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

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).
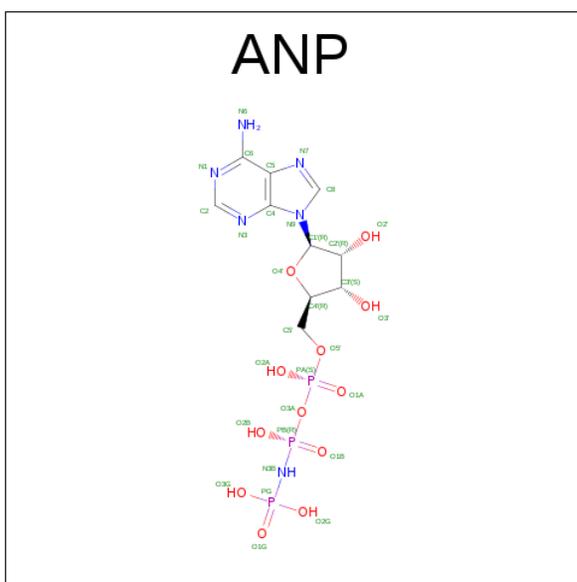
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			1	1		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: ATP-DEPENDENT RNA HELICASE DDX48

- Molecule 1: ATP-DEPENDENT RNA HELICASE DDX48

- Molecule 2: PROTEIN MAGO NASHI HOMOLOG

- Molecule 2: PROTEIN MAGO NASHI HOMOLOG

MET GLU SER D4 F5 Y6 Y10 H13 K16 F17 E20 F21 L22 G30 K31 L32 R33 R47 R82 Q86 E87 I90 V91 I97 S98 F99 T100 T101 I108 Q112 S135 H140 I146

• Molecule 3: RNA-BINDING PROTEIN 8A

Chain D:

6%

63% 17% • 18%

P66 Q67 R68 S69 I74 V80 H81 A84 T85 E86 H90 A94 E95 Y96 R108 T123 E126 E132 N135 G136 Q137 D138 L139 M140 S145 W148 V151 P154 PRO LYS GLY LYS ARG ARG GLY GLY ARG ARG ARG SER SER PRO ASP ARG ARG

ARG ARG

• Molecule 3: RNA-BINDING PROTEIN 8A

Chain G:

6%

68% 14% 18%

P66 Q67 R68 S69 F76 V77 A84 T85 E86 L106 T123 E126 E132 G133 L134 N135 L139 M140 S145 V146 D147 W148 V151 P154 PRO LYS GLY LYS ARG ARG GLY GLY ARG ARG ARG SER SER PRO ASP ARG ARG ARG

• Molecule 4: 5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3'

Chain E: 7% 33% 60%

U1 U2 U3 U4 U5 U6 U U U U U U U U U

• Molecule 4: 5'-R(*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3'

Chain H: 20% 7% 13% 60%

U1 U2 U3 U6 U U U U U U U U U

• Molecule 5: PROTEIN CASC3

Chain I:

8%

29% 13% 58%

ASP THR LYS SER THR VAL THR GLY GLU ARG GLN SER ASP GLY GLN GLU GLU SER THR GLU PRO VAL GLU ASN LYS VAL GLY LYS LYS GLY PRO K168 H169 L170 D171 D172 D173 E174 D175 P179 K185 L193 Q196 THR GLN GLU GLU GLU VAL ARG PRO LYS GLY ARG GLN ARG

LYS LEU TRP LYS ASP E215 G216 R217 W218 E219 F223 R224 E227 Q228 Q234 A238 L239 Y240 G241 Y242 D243 I244 H248 ASN PRO ASP ASP ILE LYS PRO ARG ARG ILE ARG LYS PRO ARG TYR GLY SER PRO PRO GLN ARG ASP PRO ASN TRP ASN GLY GLU ARG LEU ASN LYS

SER HIS ARG HIS GLN GLY

• Molecule 5: PROTEIN CASC3

Chain T:

8%

33% 8% •• 57%

ASP THR LYS SER THR VAL THR GLY GLU ARG GLN SER GLY ASP GLY GLN GLU SER THR GLU PRO VAL GLU ASN LYS VAL GLY LYS LYS GLY PRO **K168** **H169** **D172** **Q196** **T197** GLN GLU GLU GLU VAL ARG PRO LYS GLY ARG GLN ARG LYS LEU TRP LYS **D214** **E215** **G216** **R217** **R224**

E225 **D226** E227 Q228 **S232** **R233** **Q234** **E235** **L236** **I237** **A238** **L239** **Y240** **G241** **S246** **A247** **H248** ASN PRO ASP ASP ILE LYS PRO ARG ARG ILE ARG LYS PRO ARG TYR GLY SER PRO PRO GLN ARG ASP PRO ASN TRP ASN GLY GLU ARG LEU ASN LYS SER HIS ARG HIS GLN GLY

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.15Å 161.24Å 193.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.98 – 3.20 46.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.98-3.20) 95.5 (46.97-3.20)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	0.24	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.232 , 0.277 0.237 , 0.282	Depositor DCC
R_{free} test set	1746 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	56.8	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 89.5	EDS
L-test for twinning[2]	$< |L| > = 0.40, < L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11226	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.06 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.8224e-03.*

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[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: MG, ANP

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	0.46	0/3122	0.64	0/4224
1	B	0.45	0/3130	0.66	1/4233 (0.0%)
2	C	0.53	0/1207	0.62	0/1627
2	F	0.51	0/1207	0.62	0/1627
3	D	0.39	0/705	0.55	0/958
3	G	0.39	0/705	0.56	0/958
4	E	1.32	1/132 (0.8%)	1.57	3/200 (1.5%)
4	H	1.25	1/132 (0.8%)	1.44	0/200
5	I	0.48	0/507	0.66	0/684
5	T	0.51	0/551	0.70	0/740
All	All	0.50	2/11398 (0.0%)	0.67	4/15451 (0.0%)

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	1
1	B	0	2
5	T	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	U	OP3-P	-9.83	1.49	1.61
4	E	1	U	OP3-P	-9.37	1.50	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	108	GLN	N-CA-C	9.66	137.08	111.00
4	E	3	U	O4'-C1'-N1	6.01	113.01	108.20
4	E	4	U	O4'-C1'-N1	5.74	112.79	108.20
4	E	5	U	O4'-C1'-N1	5.16	112.32	108.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	408	ALA	Peptide
1	B	107	THR	Peptide
1	B	408	ALA	Peptide
5	T	247	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3073	0	3066	34	0
1	B	3081	0	3083	30	0
2	C	1178	0	1157	7	0
2	F	1178	0	1157	10	0
3	D	688	0	633	8	0
3	G	688	0	633	4	0
4	E	121	0	61	0	0
4	H	121	0	61	2	0
5	I	495	0	406	8	0
5	T	538	0	472	10	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	31	0	13	3	0
7	B	31	0	13	1	0
8	A	1	0	0	0	0
All	All	11226	0	10755	105	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 5.

The worst 5 of 105 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:408:ALA:HB3	1:B:409:ASP:HB2	1.66	0.78
1:A:408:ALA:HB3	1:A:409:ASP:HB2	1.67	0.74
1:B:121:GLN:HE21	1:B:324:ARG:HH22	1.33	0.73
1:A:121:GLN:HE21	1:A:324:ARG:HH22	1.41	0.68
1:A:107:THR:HA	1:A:108:GLN:CB	2.26	0.66

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	388/410 (95%)	360 (93%)	25 (6%)	3 (1%)	22	65
1	B	388/410 (95%)	361 (93%)	24 (6%)	3 (1%)	22	65
2	C	141/146 (97%)	129 (92%)	11 (8%)	1 (1%)	25	68
2	F	141/146 (97%)	131 (93%)	9 (6%)	1 (1%)	25	68
3	D	87/109 (80%)	80 (92%)	4 (5%)	3 (3%)	4	28
3	G	87/109 (80%)	80 (92%)	4 (5%)	3 (3%)	4	28
5	I	59/150 (39%)	46 (78%)	9 (15%)	4 (7%)	1	10
5	T	61/150 (41%)	52 (85%)	8 (13%)	1 (2%)	11	50
All	All	1352/1630 (83%)	1239 (92%)	94 (7%)	19 (1%)	13	53

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	383	ASN
1	B	108	GLN
1	B	383	ASN

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Mol	Chain	Res	Type
3	D	86	GLU

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	330/360 (92%)	308 (93%)	22 (7%)	19	56
1	B	332/360 (92%)	309 (93%)	23 (7%)	18	55
2	C	127/134 (95%)	120 (94%)	7 (6%)	25	64
2	F	127/134 (95%)	121 (95%)	6 (5%)	30	69
3	D	67/92 (73%)	61 (91%)	6 (9%)	11	40
3	G	67/92 (73%)	61 (91%)	6 (9%)	11	40
5	I	43/133 (32%)	39 (91%)	4 (9%)	10	38
5	T	52/133 (39%)	46 (88%)	6 (12%)	6	28
All	All	1145/1438 (80%)	1065 (93%)	80 (7%)	18	54

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	273	ASP
1	B	407	VAL
5	I	239	LEU
1	B	303	THR
1	B	348	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	253	GLN
1	B	351	ASN
3	G	142	GLN
1	B	308	HIS

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Mol	Chain	Res	Type
1	B	313	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	E	5/15 (33%)	1 (20%)	0
4	H	5/15 (33%)	2 (40%)	0
All	All	10/30 (33%)	3 (30%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	E	6	U
4	H	3	U
4	H	6	U

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1413	6	29,33,33	2.07	7 (24%)	28,52,52	2.12	7 (25%)
7	ANP	B	1413	6	29,33,33	2.18	10 (34%)	28,52,52	2.35	6 (21%)

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	1413	6	-	0/13/38/38	0/3/3/3
7	ANP	B	1413	6	-	0/13/38/38	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1413	ANP	PB-O2B	-2.47	1.49	1.56
7	B	1413	ANP	PG-O2G	-2.24	1.50	1.56
7	A	1413	ANP	PG-O2G	-2.24	1.50	1.56
7	B	1413	ANP	PG-O3G	-2.20	1.50	1.56
7	B	1413	ANP	O4'-C1'	2.10	1.44	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1413	ANP	N3-C2-N1	-6.73	123.00	128.86
7	B	1413	ANP	N3-C2-N1	-6.36	123.32	128.86
7	B	1413	ANP	O1B-PB-N3B	-6.14	102.61	111.79
7	B	1413	ANP	O1G-PG-N3B	-4.38	105.23	111.79
7	A	1413	ANP	O1B-PB-N3B	-3.46	106.61	111.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1413	ANP	3	0
7	B	1413	ANP	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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(Å²)	Q<0.9
1	A	390/410 (95%)	0.07	3 (0%)	86	77	56, 69, 84, 90	0
1	B	390/410 (95%)	0.21	6 (1%)	74	61	56, 69, 83, 90	0
2	C	143/146 (97%)	-0.15	0	100	100	54, 62, 71, 74	0
2	F	143/146 (97%)	-0.02	0	100	100	54, 62, 71, 74	0
3	D	89/109 (81%)	0.63	7 (7%)	13	7	65, 75, 89, 93	0
3	G	89/109 (81%)	0.56	6 (6%)	19	10	65, 75, 89, 93	0
4	E	6/15 (40%)	-0.54	0	100	100	40, 44, 58, 68	0
4	H	6/15 (40%)	-0.21	0	100	100	55, 63, 73, 81	0
5	I	63/150 (42%)	0.85	12 (19%)	1	1	67, 80, 97, 100	0
5	T	65/150 (43%)	0.85	12 (18%)	1	1	53, 74, 82, 83	0
All	All	1384/1660 (83%)	0.21	46 (3%)	47	31	40, 69, 85, 100	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	T	197	THR	5.6
1	B	276	THR	4.2
5	I	169	HIS	3.9
5	I	172	ASP	3.7
5	I	215	GLU	3.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

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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, 95th 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	B	1412	1/1	0.95	0.34	2.09	19,19,19,19	0
7	ANP	A	1413	31/31	0.92	0.19	-0.94	47,48,52,52	0
7	ANP	B	1413	31/31	0.93	0.20	-1.15	37,41,50,51	0
6	MG	A	1412	1/1	0.92	0.28	-	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.