



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:52 PM GMT

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

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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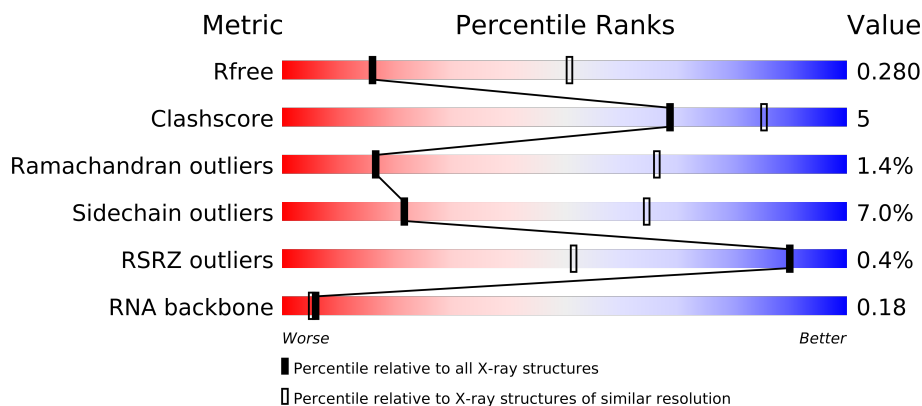
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	410	
1	B	410	
2	C	146	
2	F	146	
3	D	109	
3	G	109	
4	E	15	
4	H	15	
5	I	150	
5	T	150	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	MG	A	1412	-	X
6	MG	B	1412	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11226 atoms, of which 0 are hydrogen and 0 are deuterium.

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\*UP\*U P\*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			

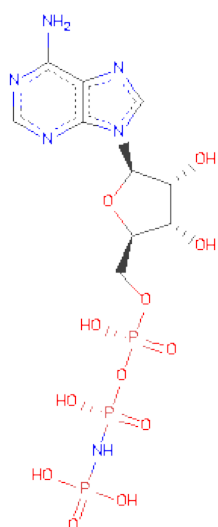
- Molecule 5 is a protein called PROTEIN CASC3.

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 PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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.

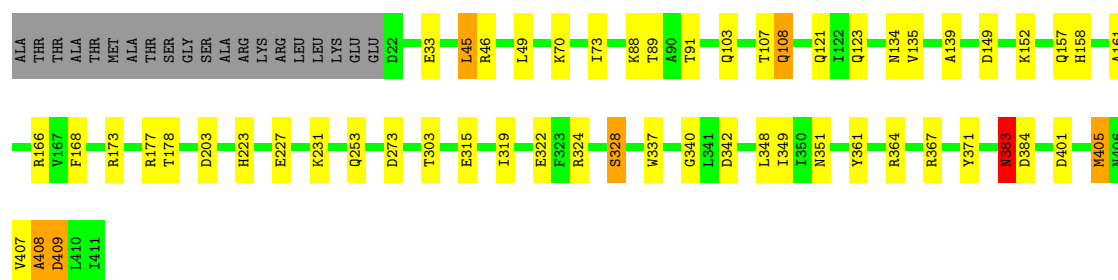
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			1	1		

### 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 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.

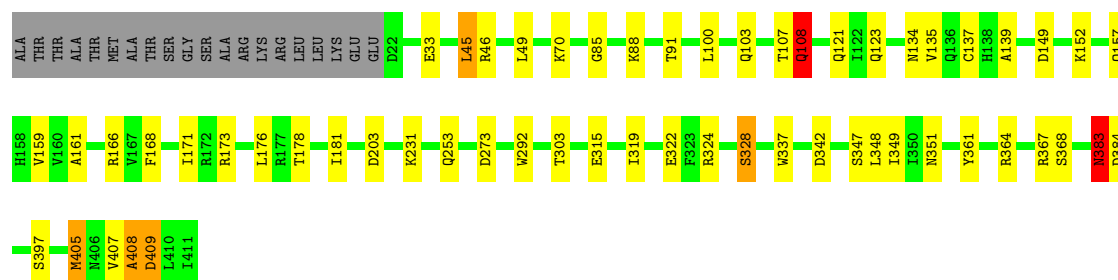
#### • Molecule 1: ATP-DEPENDENT RNA HELICASE DDX48

Chain A:



#### • Molecule 1: ATP-DEPENDENT RNA HELICASE DDX48

Chain B:



#### • Molecule 2: PROTEIN MAGO NASHI HOMOLOG

Chain C:



#### • Molecule 2: PROTEIN MAGO NASHI HOMOLOG

Chain F:



#### • Molecule 3: RNA-BINDING PROTEIN 8A

Chain D:



- Molecule 3: RNA-BINDING PROTEIN 8A

Chain G: 



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

Chain E: 



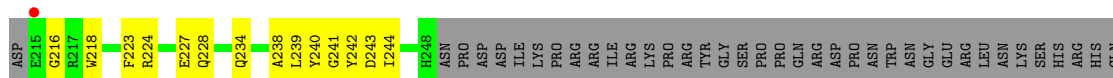
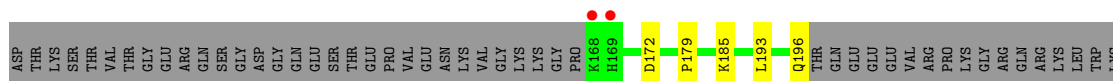
● Molecule 4: 5'-R(\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*UP\*U)-3'

Chain H:



- Molecule 5: PROTEIN CASC3

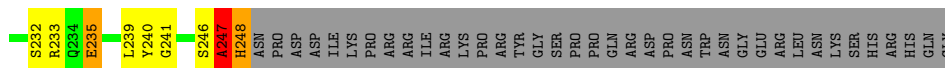
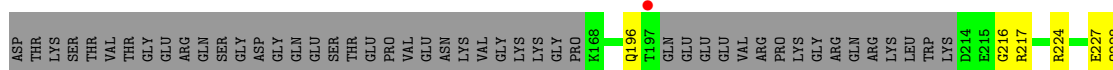
Chain I:



GLY

- Molecule 5: PROTEIN CASC3

Chain T: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.232 , 0.277 0.238 , 0.280	Depositor DCC
$R_{free}$ test set	1746 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 34926 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	11226	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

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



## 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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 5.

All (105) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:351:ASN:HD21	1:A:364:ARG:HD3	1.60	0.66
5:I:240:TYR:H	5:I:241:GLY:HA2	1.65	0.62
1:B:253:GLN:NE2	1:B:361:TYR:OH	2.32	0.61
1:B:349:ILE:HD11	1:B:367:ARG:HB2	1.84	0.60
1:A:383:ASN:HD22	1:A:384:ASP:H	1.49	0.59
1:B:139:ALA:HA	1:B:161:ALA:O	2.03	0.59
1:A:108:GLN:CB	1:A:158:HIS:O	2.52	0.58
1:B:85:GLY:N	7:B:1413:ANP:O3G	2.37	0.58
1:A:349:ILE:HD11	1:A:367:ARG:HB2	1.86	0.58
1:B:351:ASN:HD21	1:B:364:ARG:HD3	1.68	0.58
3:D:66:PRO:HB3	3:D:148:TRP:CD2	2.40	0.56
1:A:253:GLN:NE2	1:A:361:TYR:OH	2.38	0.56
5:I:240:TYR:N	5:I:241:GLY:HA2	2.22	0.55
1:B:408:ALA:CB	1:B:409:ASP:HB2	2.35	0.55
1:A:401:ASP:OD2	3:D:108:ARG:NH2	2.40	0.55
1:A:139:ALA:HA	1:A:161:ALA:O	2.07	0.54
1:B:121:GLN:NE2	1:B:324:ARG:HH22	2.05	0.53
1:B:383:ASN:HD22	1:B:384:ASP:H	1.56	0.53
1:A:408:ALA:CB	1:A:409:ASP:HB2	2.36	0.52
5:T:240:TYR:H	5:T:241:GLY:HA2	1.75	0.52
3:G:66:PRO:HB3	3:G:148:TRP:CD2	2.45	0.52
5:T:246:SER:O	5:T:247:ALA:HB2	2.10	0.52
1:A:33:GLU:N	1:A:33:GLU:OE2	2.42	0.52
1:B:33:GLU:OE2	1:B:33:GLU:N	2.42	0.51
5:I:227:GLU:O	5:I:228:GLN:NE2	2.44	0.51
5:T:247:ALA:O	5:T:248:HIS:HB3	2.10	0.50
4:H:6:U:C6	4:H:6:U:H5"	2.46	0.50
2:F:86:GLN:N	2:F:101:THR:O	2.42	0.50
1:B:108:GLN:HA	1:B:181:ILE:HA	1.93	0.49
1:A:351:ASN:ND2	1:A:364:ARG:HD3	2.27	0.49
1:A:351:ASN:HD21	1:A:364:ARG:CD	2.25	0.49
1:A:231:LYS:O	5:T:217:ARG:HG2	2.12	0.49
1:B:408:ALA:CA	1:B:409:ASP:HB2	2.43	0.48
3:G:123:THR:OG1	3:G:126:GLU:HG2	2.13	0.48
1:A:408:ALA:CA	1:A:409:ASP:HB2	2.44	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:90:ILE:HB	2:F:97:ILE:HG13	1.94	0.48
1:A:322:GLU:HB3	1:A:328:SER:HB2	1.96	0.48
1:B:405:MET:CE	1:B:405:MET:H	2.26	0.48
1:A:315:GLU:O	1:A:319:ILE:HG12	2.14	0.48
1:A:340:GLY:HA2	7:A:1413:ANP:O2G	2.13	0.47
1:B:315:GLU:O	1:B:319:ILE:HG12	2.13	0.47
1:B:100:LEU:HD22	1:B:108:GLN:HG3	1.96	0.47
2:C:90:ILE:HB	2:C:97:ILE:HG13	1.95	0.47
1:A:405:MET:CE	1:A:405:MET:H	2.27	0.47
4:H:3:U:H6	4:H:3:U:H5"	1.80	0.47
1:B:351:ASN:HD22	1:B:364:ARG:HH11	1.63	0.46
1:A:88:LYS:O	1:A:91:THR:HB	2.15	0.46
1:A:351:ASN:ND2	1:A:364:ARG:HH11	2.14	0.46
1:B:88:LYS:O	1:B:91:THR:HB	2.16	0.46
5:I:242:TYR:O	5:I:244:ILE:N	2.49	0.45
1:A:45:LEU:HD13	1:A:49:LEU:HD23	1.98	0.45
2:C:86:GLN:N	2:C:101:THR:O	2.45	0.45
1:A:121:GLN:HE22	1:A:342:ASP:H	1.65	0.45
1:B:45:LEU:HD13	1:B:49:LEU:HD23	1.99	0.45
2:F:97:ILE:HD13	2:F:99:PHE:CE2	2.52	0.45
2:F:108:ILE:O	2:F:112:GLN:HG2	2.17	0.45
1:A:383:ASN:ND2	1:A:384:ASP:H	2.15	0.44
5:T:240:TYR:N	5:T:241:GLY:HA2	2.32	0.44
1:B:137:CYS:SG	1:B:159:VAL:HB	2.58	0.44
1:A:349:ILE:HD13	1:A:364:ARG:O	2.18	0.44
1:A:223:HIS:ND1	1:A:227:GLU:OE2	2.46	0.44
5:I:223:PHE:CE2	5:I:228:GLN:HG3	2.52	0.44
2:F:6:TYR:HB3	2:F:91:VAL:HB	2.00	0.44
3:D:123:THR:OG1	3:D:126:GLU:HG2	2.18	0.44
1:B:351:ASN:ND2	1:B:364:ARG:HD3	2.33	0.43
2:F:90:ILE:HD12	2:F:97:ILE:HD11	2.00	0.43
5:T:232:SER:O	5:T:235:GLU:N	2.51	0.43
2:F:16:LYS:HE2	2:F:17:PHE:CZ	2.53	0.43
1:A:121:GLN:NE2	1:A:324:ARG:HH22	2.14	0.43
3:D:96:TYR:O	3:D:126:GLU:HB2	2.18	0.43
3:D:90:HIS:O	3:D:94:ALA:HB2	2.19	0.43
1:B:349:ILE:HD13	1:B:364:ARG:O	2.19	0.43
1:B:121:GLN:HE22	1:B:342:ASP:H	1.67	0.43
1:B:347:SER:HA	1:B:368:SER:HB2	2.01	0.43
5:T:239:LEU:HD23	5:T:239:LEU:H	1.84	0.42
1:B:292:TRP:HB2	5:I:179:PRO:HB2	2.01	0.42
1:A:351:ASN:HD22	1:A:364:ARG:HH11	1.65	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:13:HIS:CE1	2:F:20:GLU:HB2	2.55	0.42
5:T:235:GLU:O	5:T:239:LEU:HD23	2.19	0.42
2:C:139:LEU:HB3	3:D:74:ILE:HD11	2.01	0.42
1:B:168:PHE:CE1	1:B:203:ASP:HB3	2.55	0.42
1:A:89:THR:OG1	7:A:1413:ANP:O1B	2.38	0.42
2:C:97:ILE:HD13	2:C:99:PHE:CE2	2.54	0.42
1:B:231:LYS:HD2	5:I:216:GLY:HA3	2.02	0.42
1:B:322:GLU:HB3	1:B:328:SER:HB2	2.01	0.42
5:T:216:GLY:HA2	5:T:217:ARG:HA	1.88	0.41
2:F:10:TYR:HB3	2:F:87:GLU:HB2	2.02	0.41
1:B:408:ALA:N	1:B:409:ASP:CB	2.83	0.41
2:C:140:HIS:HA	3:D:69:SER:HB3	2.02	0.41
2:C:6:TYR:HB3	2:C:91:VAL:HB	2.03	0.41
1:A:408:ALA:N	1:A:409:ASP:CB	2.83	0.41
3:G:106:LEU:N	3:G:106:LEU:HD12	2.36	0.41
2:C:90:ILE:HD12	2:C:97:ILE:HD11	2.02	0.41
1:A:177:ARG:HB2	5:T:228:GLN:NE2	2.35	0.41
2:F:140:HIS:HA	3:G:69:SER:HB3	2.02	0.41
3:D:138:ASP:O	3:D:139:LEU:HD12	2.21	0.40
1:A:371:TYR:CE2	7:A:1413:ANP:C2	3.04	0.40
5:I:234:GLN:O	5:I:238:ALA:N	2.54	0.40
1:B:171:ILE:HA	1:B:176:LEU:O	2.21	0.40
1:A:168:PHE:CE1	1:A:203:ASP:HB3	2.57	0.40

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%)	27 77
1	B	388/410 (95%)	361 (93%)	24 (6%)	3 (1%)	27 77
2	C	141/146 (97%)	129 (92%)	11 (8%)	1 (1%)	30 80
2	F	141/146 (97%)	131 (93%)	9 (6%)	1 (1%)	30 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	87/109 (80%)	80 (92%)	4 (5%)	3 (3%)	6	38
3	G	87/109 (80%)	80 (92%)	4 (5%)	3 (3%)	6	38
5	I	59/150 (39%)	46 (78%)	9 (15%)	4 (7%)	2	15
5	T	61/150 (41%)	52 (85%)	8 (13%)	1 (2%)	14	63
All	All	1352/1630 (83%)	1239 (92%)	94 (7%)	19 (1%)	16	66

All (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
3	D	86	GLU
3	G	86	GLU
5	T	247	ALA
2	C	30	GLY
3	D	84	ALA
2	F	30	GLY
3	G	84	ALA
3	G	135	ASN
5	I	185	LYS
5	I	243	ASP
1	A	409	ASP
1	B	409	ASP
3	D	135	ASN
5	I	172	ASP
5	I	218	TRP

### 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%)	23	66
1	B	332/360 (92%)	309 (93%)	23 (7%)	22	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	127/134 (95%)	120 (94%)	7 (6%)	30	75
2	F	127/134 (95%)	121 (95%)	6 (5%)	36	79
3	D	67/92 (73%)	61 (91%)	6 (9%)	14	49
3	G	67/92 (73%)	61 (91%)	6 (9%)	14	49
5	I	43/133 (32%)	39 (91%)	4 (9%)	13	46
5	T	52/133 (39%)	46 (88%)	6 (12%)	8	35
All	All	1145/1438 (80%)	1065 (93%)	80 (7%)	21	64

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	46	ARG
1	A	70	LYS
1	A	73	ILE
1	A	103	GLN
1	A	123	GLN
1	A	134	ASN
1	A	135	VAL
1	A	149	ASP
1	A	152	LYS
1	A	157	GLN
1	A	166	ARG
1	A	173	ARG
1	A	178	THR
1	A	273	ASP
1	A	303	THR
1	A	328	SER
1	A	337	TRP
1	A	348	LEU
1	A	383	ASN
1	A	405	MET
1	A	407	VAL
1	B	45	LEU
1	B	46	ARG
1	B	70	LYS
1	B	103	GLN
1	B	108	GLN
1	B	123	GLN
1	B	134	ASN

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Mol	Chain	Res	Type
1	B	135	VAL
1	B	149	ASP
1	B	152	LYS
1	B	157	GLN
1	B	166	ARG
1	B	173	ARG
1	B	178	THR
1	B	273	ASP
1	B	303	THR
1	B	328	SER
1	B	337	TRP
1	B	348	LEU
1	B	383	ASN
1	B	397	SER
1	B	405	MET
1	B	407	VAL
2	C	7	LEU
2	C	22	LEU
2	C	32	LEU
2	C	33	ARG
2	C	47	ARG
2	C	82	ARG
2	C	135	SER
3	D	67	GLN
3	D	132	GLU
3	D	139	LEU
3	D	140	MET
3	D	145	SER
3	D	151	VAL
2	F	22	LEU
2	F	32	LEU
2	F	33	ARG
2	F	47	ARG
2	F	82	ARG
2	F	135	SER
3	G	67	GLN
3	G	132	GLU
3	G	139	LEU
3	G	140	MET
3	G	145	SER
3	G	151	VAL
5	I	193	LEU

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Mol	Chain	Res	Type
5	I	196	GLN
5	I	224	ARG
5	I	239	LEU
5	T	196	GLN
5	T	224	ARG
5	T	227	GLU
5	T	233	ARG
5	T	235	GLU
5	T	248	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	157	GLN
1	A	253	GLN
1	A	308	HIS
1	A	313	GLN
1	A	351	ASN
1	A	356	ASN
1	A	383	ASN
1	B	121	GLN
1	B	157	GLN
1	B	253	GLN
1	B	308	HIS
1	B	313	GLN
1	B	351	ASN
1	B	356	ASN
1	B	383	ASN
2	C	86	GLN
3	D	137	GLN
3	D	142	GLN
2	F	13	HIS
2	F	86	GLN
3	G	137	GLN
3	G	142	GLN
5	I	196	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	33,33,33	3.27	6 (18%)	51,52,52	2.08	13 (25%)
7	ANP	B	1413	6	33,33,33	3.09	6 (18%)	51,52,52	2.64	11 (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	-	0/18/38/38	0/1/3/3
7	ANP	B	1413	6	-	0/18/38/38	0/1/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1413	ANP	PG-N3B	12.01	1.74	1.64
7	A	1413	ANP	PB-N3B	11.11	1.74	1.64
7	B	1413	ANP	PG-N3B	11.04	1.73	1.64
7	B	1413	ANP	PB-N3B	10.03	1.73	1.64
7	B	1413	ANP	PG-O1G	5.48	1.52	1.46
7	A	1413	ANP	PG-O1G	4.94	1.52	1.46
7	A	1413	ANP	PB-O1B	3.99	1.51	1.46
7	B	1413	ANP	PB-O1B	3.88	1.51	1.46
7	B	1413	ANP	C5-C4	3.66	1.48	1.40
7	A	1413	ANP	C4-N9	-3.37	1.32	1.37
7	A	1413	ANP	C5-C4	3.04	1.47	1.40
7	B	1413	ANP	PB-O3A	2.59	1.62	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1413	ANP	PB-N3B-PG	-10.68	112.11	130.07
7	A	1413	ANP	N3-C2-N1	-6.83	123.00	128.71
7	B	1413	ANP	N3-C2-N1	-6.45	123.32	128.71
7	A	1413	ANP	PB-N3B-PG	-6.36	119.38	130.07
7	B	1413	ANP	O1B-PB-N3B	-6.10	102.61	111.83
7	B	1413	ANP	N3-C4-N9	5.38	135.15	125.43
7	B	1413	ANP	O4'-C1'-N9	5.38	113.44	108.44
7	A	1413	ANP	N3-C4-N9	4.85	134.18	125.43
7	B	1413	ANP	O1G-PG-N3B	-4.37	105.23	111.83
7	A	1413	ANP	O2B-PB-O1B	3.88	118.85	109.89
7	B	1413	ANP	O2B-PB-O1B	3.77	118.59	109.89
7	B	1413	ANP	C5-C4-N3	-3.52	118.04	125.70
7	A	1413	ANP	O1B-PB-N3B	-3.45	106.61	111.83
7	A	1413	ANP	O1G-PG-N3B	-3.39	106.71	111.83
7	B	1413	ANP	O3A-PB-N3B	3.16	115.35	106.59
7	B	1413	ANP	C4-C5-N7	-3.09	106.87	109.52
7	A	1413	ANP	C4-C5-N7	-2.82	107.11	109.52
7	A	1413	ANP	C5-C4-N3	-2.73	119.75	125.70
7	A	1413	ANP	PA-O3A-PB	-2.66	122.71	131.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1413	ANP	C8-N9-C4	2.66	108.93	106.90
7	B	1413	ANP	C2-N3-C4	2.51	121.15	114.01
7	A	1413	ANP	O4'-C1'-N9	2.37	110.64	108.44
7	A	1413	ANP	C2-N3-C4	2.21	120.30	114.01
7	A	1413	ANP	C2-N1-C6	2.14	122.63	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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	390/410 (95%)	-0.10	0	100	100	56, 69, 84, 90	0
1	B	390/410 (95%)	-0.06	0	100	100	56, 69, 83, 90	0
2	C	143/146 (97%)	-0.21	0	100	100	54, 62, 71, 74	0
2	F	143/146 (97%)	-0.14	0	100	100	54, 62, 71, 74	0
3	D	89/109 (81%)	0.23	0	100	100	65, 75, 89, 93	0
3	G	89/109 (81%)	0.23	1 (1%)	77	27	65, 75, 89, 93	0
4	E	6/15 (40%)	-0.64	0	100	100	40, 44, 58, 68	0
4	H	6/15 (40%)	-0.46	0	100	100	55, 63, 73, 81	0
5	I	63/150 (42%)	0.29	3 (4%)	29	6	67, 80, 97, 100	0
5	T	65/150 (43%)	0.23	1 (1%)	70	21	53, 74, 82, 83	0
All	All	1384/1660 (83%)	-0.03	5 (0%)	90	51	40, 69, 85, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	154	PRO	2.3
5	I	168	LYS	2.2
5	I	215	GLU	2.2
5	I	169	HIS	2.1
5	T	197	THR	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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<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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	B	1412	1/1	0.42	4.00	19,19,19,19	0
6	MG	A	1412	1/1	0.33	2.30	25,25,25,25	0
7	ANP	A	1413	31/31	0.22	0.03	47,48,52,52	0
7	ANP	B	1413	31/31	0.23	-0.32	37,41,50,51	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.