



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:49 AM UTC

PDB ID : 2J0S / pdb_00002j0s
Title : The crystal structure of the Exon Junction Complex at 2.2 Å resolution
Authors : Bono, F.; Ebert, J.; Lorentzen, E.; Conti, E.
Deposited on : 2006-08-04
Resolution : 2.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

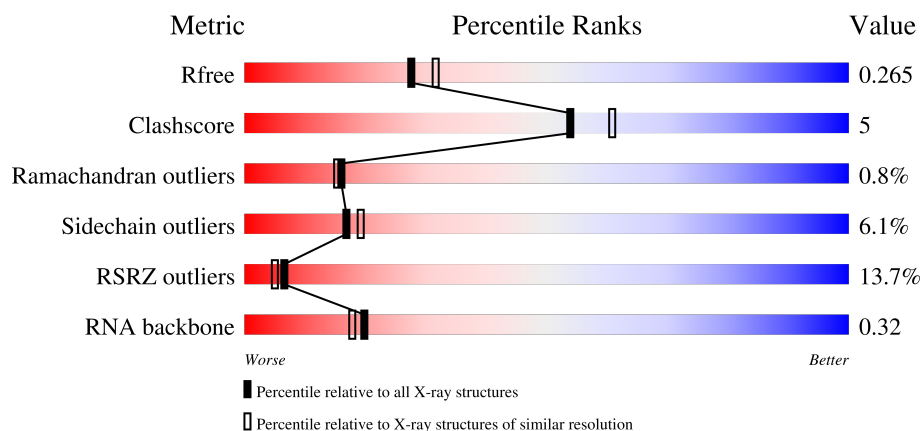
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)
RNA backbone	3983	1098 (2.54-1.90)

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 $\leq 5\%$. 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	15% 82% 10% 5%
2	C	146	8% 86% 11% ••
3	D	89	15% 85% 13% •
4	E	15	27% 13% 60%

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Mol	Chain	Length	Quality of chain
5	T	150	 A horizontal bar chart showing the quality of chain T. The bar is divided into four segments: a small red segment at the beginning labeled '4%', followed by a green segment labeled '23%', a yellow segment labeled '6%', and a long grey segment at the end labeled '71%'. The segments are separated by thin white lines.

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5906 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	391	Total	C	N	O	S	0	8	0
			3138	1986	540	591	21			

- 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	2	0
			1192	773	199	217	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	1	0
			710	453	116	138	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			

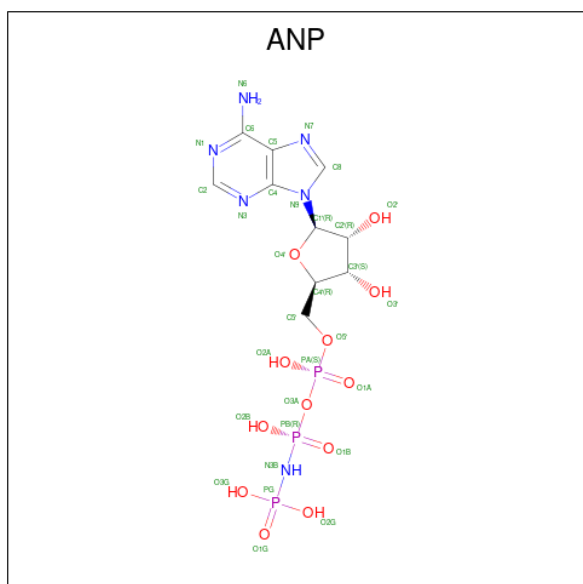
- Molecule 5 is a protein called PROTEIN CASC3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	T	44	Total	C	N	O	0	0	0
			369	228	69	72			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

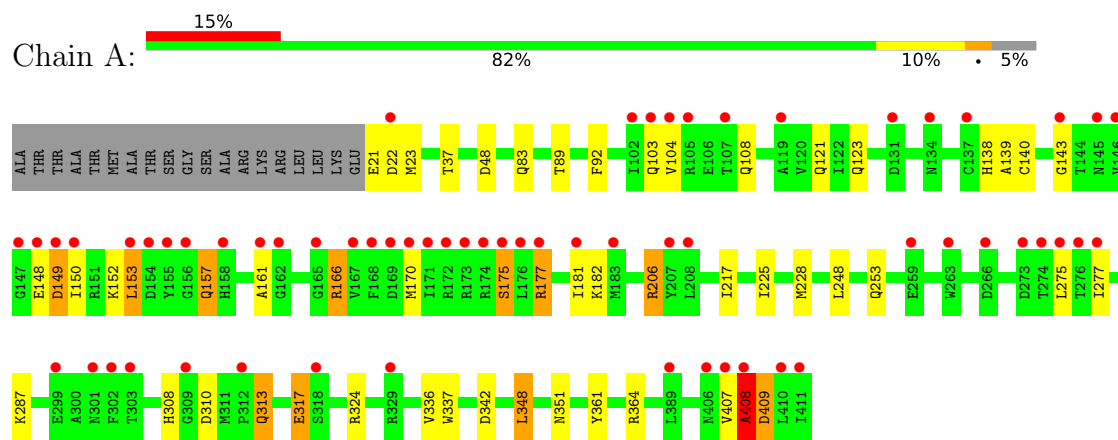
- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



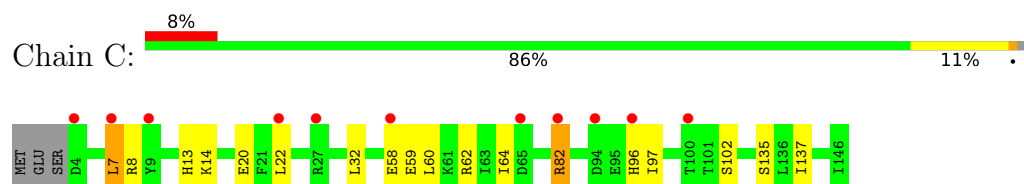
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

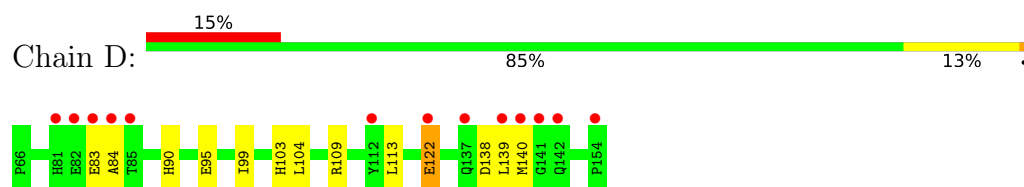
- Molecule 1: ATP-DEPENDENT RNA HELICASE DDX48



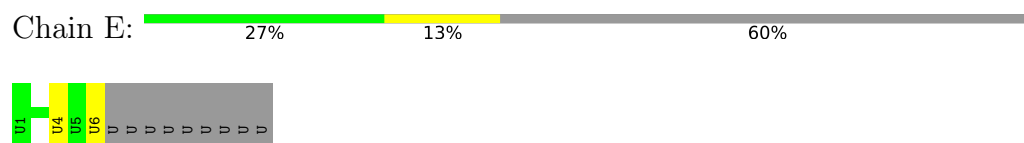
- Molecule 2: PROTEIN MAGO NASHI HOMOLOG



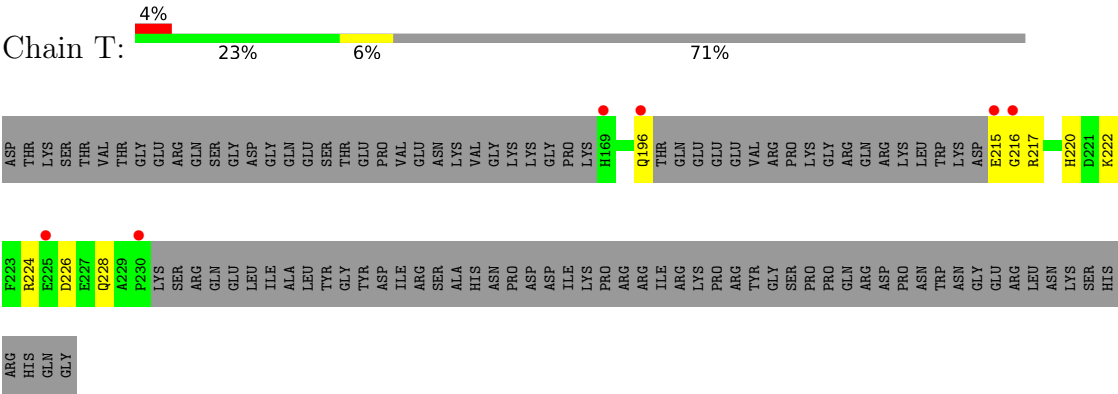
- Molecule 3: RNA-BINDING PROTEIN 8A



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



- Molecule 5: PROTEIN CASC3



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	169.44Å 169.44Å 71.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.73 – 2.21 43.73 – 2.21	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.73-2.21) 99.9 (43.73-2.21)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.185 , 0.216 0.238 , 0.265	Depositor DCC
R_{free} test set	2931 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5906	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ANP, MG

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	0.78	0/3211	0.92	4/4340 (0.1%)
2	C	0.94	0/1228	0.92	0/1655
3	D	0.76	0/730	0.86	0/989
4	E	0.86	0/132	1.44	3/200 (1.5%)
5	T	0.76	0/379	0.79	0/510
All	All	0.82	0/5680	0.92	7/7694 (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	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	6	U	O5'-C5'-C4'	6.48	121.42	111.70
4	E	6	U	O4'-C4'-C3'	-5.97	100.13	106.10
1	A	37	THR	CA-C-N	5.92	125.54	119.56
1	A	37	THR	C-N-CA	5.92	125.54	119.56
1	A	408	ALA	CA-C-N	5.49	131.58	121.70
1	A	408	ALA	C-N-CA	5.49	131.58	121.70
4	E	4	U	O3'-P-O5'	-5.35	95.97	104.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ARG	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	3138	0	3166	39	0
2	C	1192	0	1173	8	0
3	D	710	0	662	6	0
4	E	121	0	61	0	0
5	T	369	0	308	4	0
6	A	1	0	0	0	0
7	A	31	0	13	0	0
8	A	168	0	0	0	0
8	C	117	0	0	2	0
8	D	46	0	0	0	0
8	E	4	0	0	0	0
8	T	9	0	0	0	0
All	All	5906	0	5383	54	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.

All (54) 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:121:GLN:HE22	1:A:342:ASP:H	1.29	0.80
1:A:121:GLN:HE21	1:A:324:ARG:HH22	1.35	0.72
1:A:275:LEU:HD23	1:A:348[B]:LEU:CD2	2.18	0.72
2:C:102[A]:SER:OG	8:C:2087:HOH:O	2.08	0.70
1:A:275:LEU:HD23	1:A:348[B]:LEU:HD21	1.74	0.68
1:A:150:ILE:HG23	1:A:175:SER:OG	1.95	0.67
1:A:108:GLN:OE1	1:A:182:LYS:NZ	2.18	0.66
3:D:84:ALA:HA	3:D:140:MET:HE1	1.78	0.65
3:D:104:LEU:HD11	3:D:113:LEU:HD13	1.79	0.65
1:A:150:ILE:HG13	1:A:170:MET:HE1	1.87	0.57
1:A:149:ASP:HB3	1:A:170:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:HD23	1:A:348[B]:LEU:HD23	1.87	0.56
1:A:408:ALA:HB3	1:A:409:ASP:HB2	1.88	0.56
1:A:408:ALA:N	1:A:409:ASP:HB2	2.21	0.55
2:C:14:LYS:O	2:C:82:ARG:NH1	2.41	0.54
1:A:121:GLN:HE22	1:A:342:ASP:N	2.03	0.53
2:C:7:LEU:HD12	2:C:8:ARG:N	2.24	0.53
1:A:408:ALA:HB3	1:A:409:ASP:CB	2.40	0.52
2:C:137:ILE:HD11	8:C:2039:HOH:O	2.09	0.52
3:D:84:ALA:HA	3:D:140:MET:CE	2.40	0.51
1:A:206:ARG:HD3	5:T:222:LYS:HG3	1.92	0.50
1:A:351:ASN:ND2	1:A:364:ARG:HD3	2.26	0.50
1:A:121:GLN:NE2	1:A:342:ASP:H	2.06	0.50
1:A:150:ILE:CG1	1:A:170:MET:HE1	2.42	0.49
1:A:408:ALA:CA	1:A:409:ASP:HB2	2.41	0.49
1:A:21:GLU:HA	1:A:22:ASP:C	2.38	0.49
2:C:59:GLU:OE2	2:C:62:ARG:NH1	2.48	0.47
1:A:140[B]:CYS:SG	1:A:166:ARG:HG3	2.55	0.47
2:C:135:SER:OG	3:D:103:HIS:HD2	1.98	0.47
1:A:138:HIS:HB2	1:A:157:GLN:HG2	1.96	0.46
5:T:224:ARG:O	5:T:228:GLN:HB2	2.16	0.46
1:A:139:ALA:HA	1:A:161:ALA:O	2.16	0.46
1:A:351:ASN:HD21	1:A:364:ARG:HD3	1.81	0.46
1:A:108:GLN:HA	1:A:181:ILE:HA	1.99	0.45
3:D:122:GLU:O	3:D:122:GLU:HG3	2.17	0.45
1:A:275:LEU:HA	1:A:348[B]:LEU:HD23	1.99	0.44
3:D:90:HIS:CD2	3:D:99:ILE:HD12	2.52	0.44
1:A:153:LEU:CD2	1:A:170:MET:HE3	2.48	0.44
1:A:206:ARG:HA	5:T:220:HIS:HA	1.99	0.43
1:A:143:GLY:HA3	1:A:313:GLN:HG3	2.00	0.43
1:A:89:THR:HA	1:A:92:PHE:CE2	2.54	0.43
1:A:308:HIS:HD2	1:A:310:ASP:H	1.67	0.43
5:T:215:GLU:O	5:T:217:ARG:N	2.52	0.43
1:A:313:GLN:O	1:A:317:GLU:HG2	2.18	0.43
1:A:351:ASN:ND2	1:A:364:ARG:HH11	2.16	0.42
1:A:138:HIS:CB	1:A:157:GLN:HG2	2.50	0.41
1:A:287:LYS:HG2	1:A:308:HIS:HB2	2.02	0.41
2:C:60:LEU:O	2:C:64:ILE:HG12	2.21	0.41
1:A:253:GLN:NE2	1:A:361:TYR:OH	2.46	0.41
1:A:225:ILE:O	1:A:228:MET:HG2	2.20	0.41
1:A:408:ALA:CB	1:A:409:ASP:HB2	2.49	0.41
1:A:153:LEU:HD23	1:A:170:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:HIS:HE1	2:C:20:GLU:OE1	2.04	0.41
1:A:83:GLN:HB3	1:A:248:LEU:HD21	2.02	0.40

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	397/410 (97%)	388 (98%)	6 (2%)	3 (1%)	16	15
2	C	143/146 (98%)	142 (99%)	1 (1%)	0	100	100
3	D	88/89 (99%)	86 (98%)	1 (1%)	1 (1%)	11	9
5	T	40/150 (27%)	36 (90%)	3 (8%)	1 (2%)	4	2
All	All	668/795 (84%)	652 (98%)	11 (2%)	5 (1%)	16	18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	ALA
1	A	409	ASP
3	D	139	LEU
1	A	23	MET
5	T	216	GLY

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	345/360 (96%)	323 (94%)	22 (6%)	16	18
2	C	130/134 (97%)	122 (94%)	8 (6%)	16	18
3	D	72/75 (96%)	66 (92%)	6 (8%)	10	10
5	T	35/133 (26%)	33 (94%)	2 (6%)	18	21
All	All	582/702 (83%)	544 (94%)	38 (6%)	17	17

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	103	GLN
1	A	104	VAL
1	A	123	GLN
1	A	148	GLU
1	A	149	ASP
1	A	152	LYS
1	A	153	LEU
1	A	157	GLN
1	A	166	ARG
1	A	175	SER
1	A	177	ARG
1	A	206	ARG
1	A	217	ILE
1	A	277	ILE
1	A	313	GLN
1	A	317	GLU
1	A	336	VAL
1	A	337	TRP
1	A	348[A]	LEU
1	A	348[B]	LEU
1	A	407	VAL
2	C	7	LEU
2	C	22	LEU
2	C	32	LEU
2	C	58	GLU
2	C	82	ARG
2	C	96[A]	HIS
2	C	96[B]	HIS
2	C	97	ILE
3	D	83[A]	GLU

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Mol	Chain	Res	Type
3	D	83[B]	GLU
3	D	95	GLU
3	D	109	ARG
3	D	122	GLU
3	D	138	ASP
5	T	196	GLN
5	T	226	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	123	GLN
1	A	157	GLN
1	A	230	ASN
1	A	308	HIS
1	A	351	ASN
1	A	356	ASN
2	C	13	HIS
2	C	37	ASN
3	D	81	HIS
3	D	90	HIS
3	D	103	HIS
3	D	128	GLN
5	T	196	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	E	5/15 (33%)	0	0

There are no RNA backbone outliers to report.

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	2.10	12 (36%)	45,52,52	2.04	13 (28%)

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	-	3/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1413	ANP	PB-O1B	5.67	1.54	1.46
7	A	1413	ANP	C5-C4	4.29	1.46	1.39
7	A	1413	ANP	PB-N3B	3.62	1.72	1.63
7	A	1413	ANP	PG-O1G	3.59	1.51	1.46
7	A	1413	ANP	PG-O2G	-3.50	1.47	1.56
7	A	1413	ANP	PG-N3B	2.94	1.71	1.63
7	A	1413	ANP	PA-O3A	2.47	1.62	1.59
7	A	1413	ANP	C4-N9	-2.43	1.32	1.37
7	A	1413	ANP	C5-N7	-2.29	1.34	1.39
7	A	1413	ANP	C8-N7	2.26	1.36	1.31
7	A	1413	ANP	PB-O2B	-2.25	1.50	1.56
7	A	1413	ANP	C5-C6	2.11	1.46	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1413	ANP	C5-C4-N3	-4.86	120.02	126.72
7	A	1413	ANP	O2B-PB-O1B	4.58	119.70	109.87
7	A	1413	ANP	N3-C4-N9	4.24	134.38	127.17
7	A	1413	ANP	N3-C2-N1	-4.14	122.31	128.58
7	A	1413	ANP	C4-N9-C8	3.91	109.84	105.74
7	A	1413	ANP	C2-N3-C4	3.77	121.03	111.83
7	A	1413	ANP	O2G-PG-O3G	3.36	116.62	107.59
7	A	1413	ANP	O1G-PG-N3B	-3.09	107.21	111.77
7	A	1413	ANP	C4-C5-N7	-3.00	107.15	110.58
7	A	1413	ANP	N9-C8-N7	-2.85	109.90	113.94
7	A	1413	ANP	C5-N7-C8	2.59	107.51	103.45
7	A	1413	ANP	C6-C5-N7	2.26	136.44	132.09
7	A	1413	ANP	O3A-PB-N3B	-2.07	100.85	106.59

There are no chirality outliers.

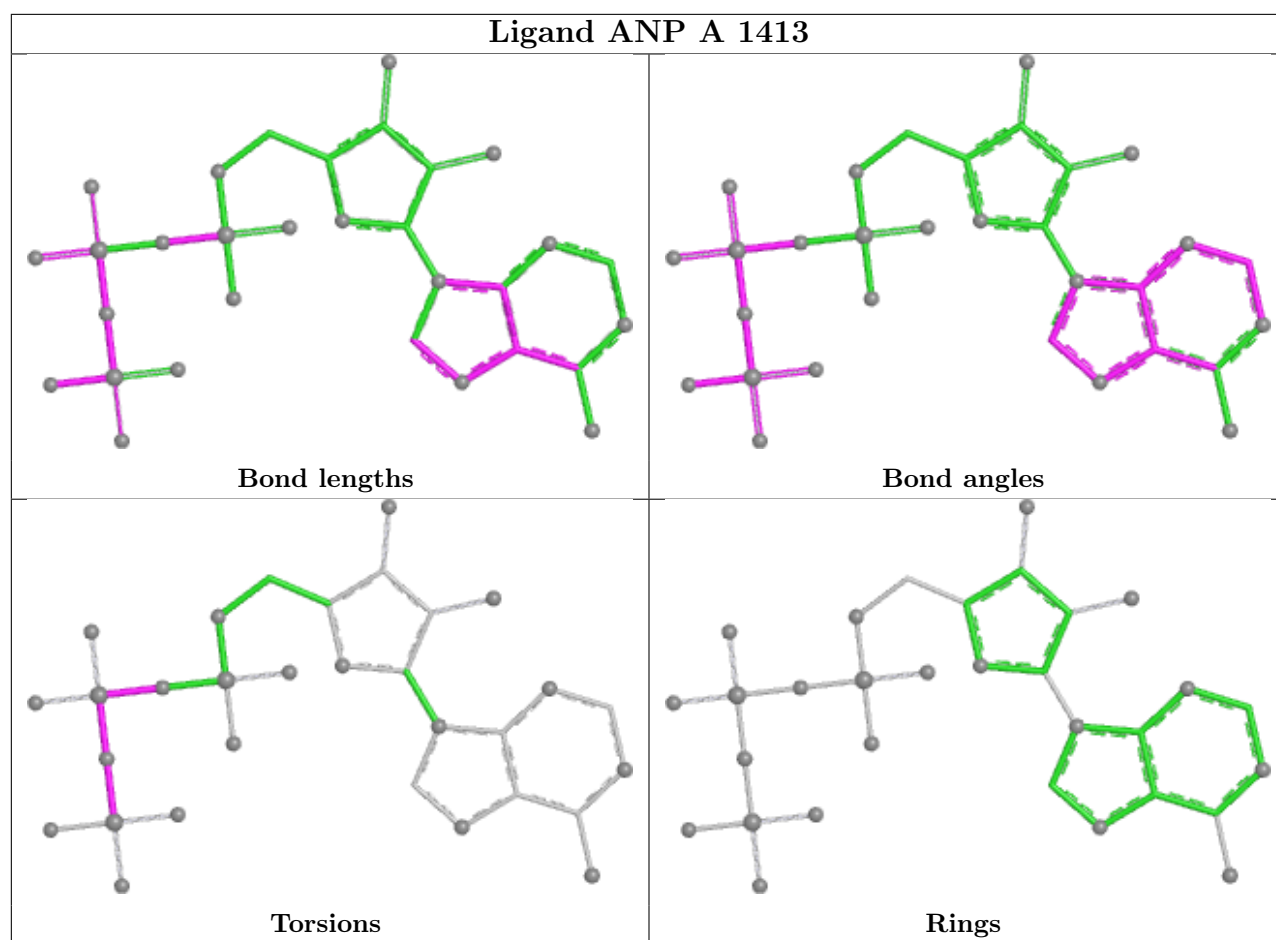
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1413	ANP	PG-N3B-PB-O1B
7	A	1413	ANP	PA-O3A-PB-O1B
7	A	1413	ANP	PB-N3B-PG-O1G

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 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(Å ²)	Q<0.9
1	A	391/410 (95%)	1.14	62 (15%) 5 4	26, 47, 57, 85	8 (2%)
2	C	143/146 (97%)	0.95	11 (7%) 19 17	29, 46, 51, 60	2 (1%)
3	D	89/89 (100%)	1.11	13 (14%) 6 4	30, 46, 54, 58	1 (1%)
4	E	6/15 (40%)	0.26	0 100 100	45, 47, 60, 82	0
5	T	44/150 (29%)	1.15	6 (13%) 7 5	36, 61, 76, 77	0
All	All	673/810 (83%)	1.09	92 (13%) 6 5	26, 47, 62, 85	11 (1%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	ILE	5.6
1	A	408	ALA	4.5
5	T	215	GLU	4.5
1	A	277	ILE	4.4
1	A	275	LEU	4.2
1	A	410	LEU	4.1
3	D	112	TYR	4.1
1	A	147	GLY	4.0
1	A	143	GLY	4.0
1	A	169	ASP	3.9
2	C	96[A]	HIS	3.8
3	D	139	LEU	3.8
1	A	156	GLY	3.8
1	A	149	ASP	3.7
1	A	407	VAL	3.7
1	A	173	ARG	3.7
3	D	140	MET	3.6
1	A	153	LEU	3.5
3	D	81	HIS	3.4
1	A	22	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	155	TYR	3.2
1	A	406	ASN	3.2
3	D	84	ALA	3.2
2	C	4	ASP	3.2
1	A	172	ARG	3.1
2	C	58	GLU	3.1
1	A	273	ASP	3.1
1	A	207	TYR	3.0
1	A	102	ILE	3.0
1	A	175	SER	3.0
1	A	103	GLN	2.9
1	A	145	ASN	2.9
5	T	196	GLN	2.9
1	A	301	ASN	2.9
5	T	230	PRO	2.8
1	A	276	THR	2.8
1	A	105	ARG	2.8
1	A	158	HIS	2.8
1	A	104	VAL	2.8
1	A	146	VAL	2.8
5	T	169	HIS	2.7
1	A	312	PRO	2.7
3	D	82	GLU	2.7
3	D	83[A]	GLU	2.7
1	A	167	VAL	2.7
1	A	177	ARG	2.7
1	A	134	ASN	2.6
1	A	154	ASP	2.6
1	A	107	THR	2.6
1	A	263	TRP	2.6
1	A	168	PHE	2.6
1	A	171	ILE	2.6
1	A	181	ILE	2.6
2	C	27	ARG	2.5
1	A	161	ALA	2.5
1	A	266	ASP	2.5
1	A	148	GLU	2.5
2	C	94	ASP	2.5
1	A	162	GLY	2.5
3	D	137	GLN	2.5
1	A	318	SER	2.4
3	D	154	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	150	ILE	2.4
3	D	122	GLU	2.4
1	A	137[A]	CYS	2.4
1	A	183	MET	2.4
2	C	82	ARG	2.4
5	T	225	GLU	2.4
1	A	329	ARG	2.3
1	A	176	LEU	2.3
1	A	303	THR	2.3
3	D	85	THR	2.3
1	A	259	GLU	2.3
2	C	65	ASP	2.2
1	A	309	GLY	2.2
1	A	174	ARG	2.2
3	D	142	GLN	2.2
1	A	119	ALA	2.2
2	C	22	LEU	2.1
1	A	170	MET	2.1
3	D	141	GLY	2.1
1	A	299	GLU	2.1
1	A	131	ASP	2.1
1	A	165	GLY	2.1
5	T	216	GLY	2.1
1	A	274	THR	2.1
2	C	100	THR	2.1
2	C	9	TYR	2.1
1	A	302	PHE	2.1
1	A	208	LEU	2.0
1	A	389	LEU	2.0
2	C	7	LEU	2.0

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 ⓘ

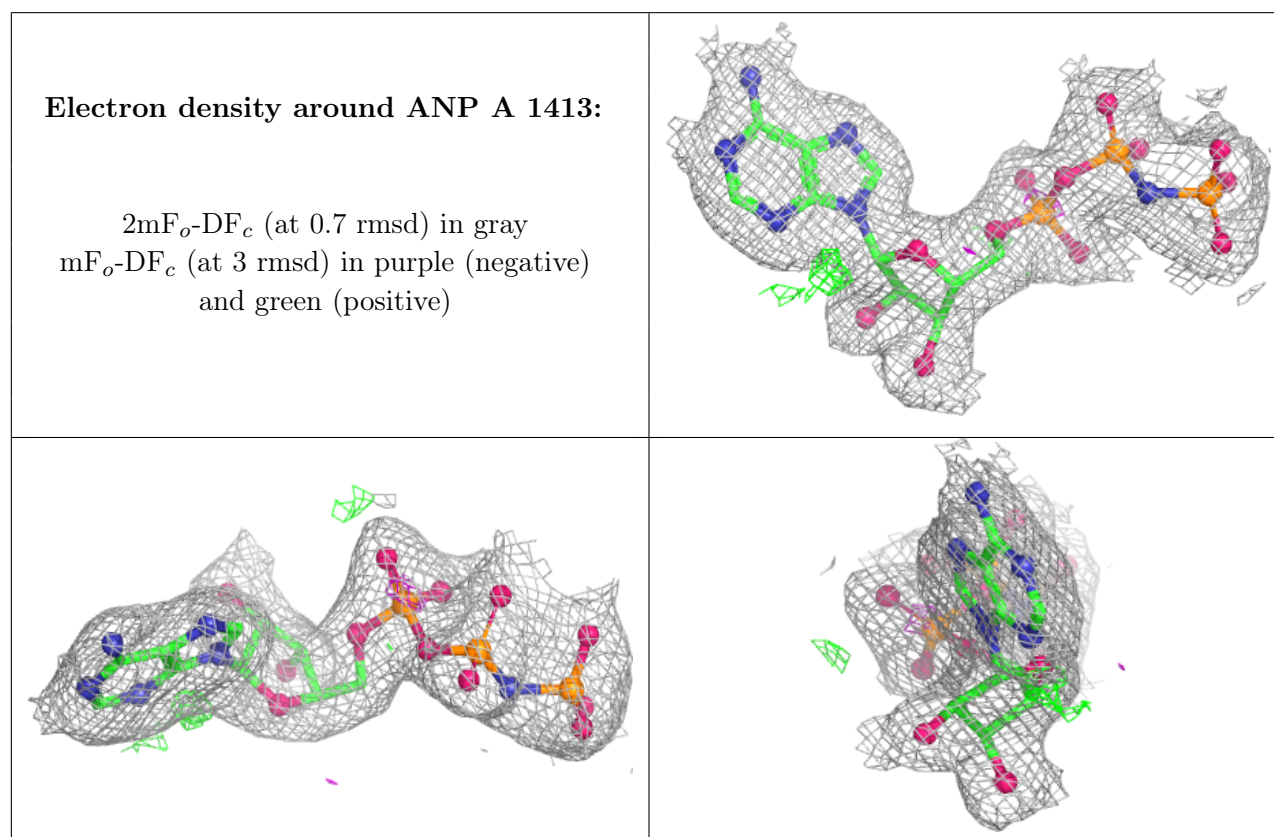
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors($\text{\AA}^2$)	Q<0.9
7	ANP	A	1413	31/31	0.98	0.07	28,32,35,37	0
6	MG	A	1412	1/1	1.00	0.05	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.