



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:16 pm BST

PDB ID : 5A4T  
Title : DYRK1A IN COMPLEX WITH NITRILE BENZOTHAZOLE FRAGMENT  
Authors : Rothweiler, U.  
Deposited on : 2015-06-15  
Resolution : 2.15 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

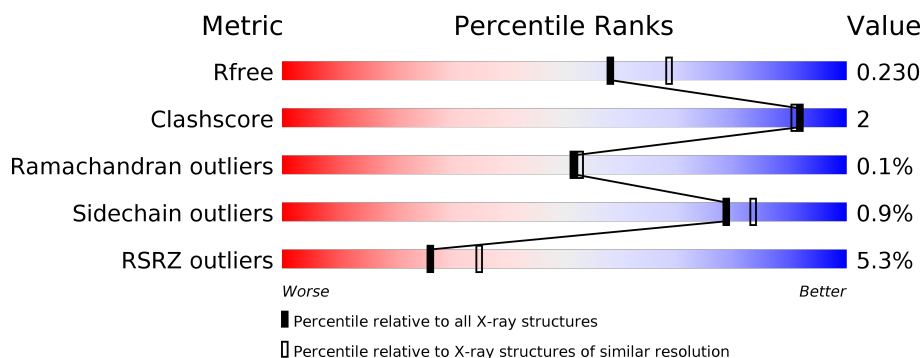
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 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	368	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> </div> </div>
1	B	368	<div> <div>6%</div> <div> <div></div> <div>88%</div> <div>8%</div> </div> </div>
1	C	368	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>10%</div> </div> </div>
1	D	368	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11182 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.

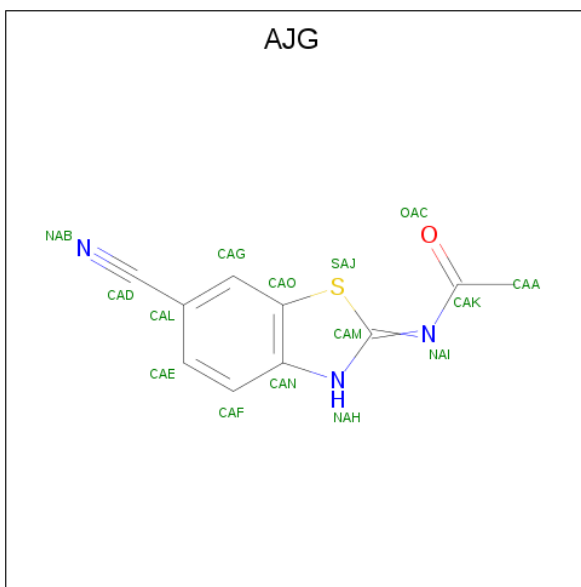
- Molecule 1 is a protein called DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	P	S	0	0	0
			2794	1798	477	501	1	17			
1	B	340	Total	C	N	O	P	S	0	0	0
			2761	1777	471	495	1	17			
1	C	333	Total	C	N	O	P	S	0	0	0
			2678	1724	452	484	1	17			
1	D	333	Total	C	N	O	P	S	0	0	0
			2711	1752	455	486	1	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLY	-	expression tag	UNP Q13627
A	124	ALA	-	expression tag	UNP Q13627
A	125	SER	-	expression tag	UNP Q13627
B	123	GLY	-	expression tag	UNP Q13627
B	124	ALA	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
C	123	GLY	-	expression tag	UNP Q13627
C	124	ALA	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
D	123	GLY	-	expression tag	UNP Q13627
D	124	ALA	-	expression tag	UNP Q13627
D	125	SER	-	expression tag	UNP Q13627

- Molecule 2 is N-(6-CYANO-3H-1,3-BENZOTHAZOL-2-YLIDENE)ETHANAMIDE (three-letter code: AJG) (formula: C<sub>10</sub>H<sub>7</sub>N<sub>3</sub>OS).

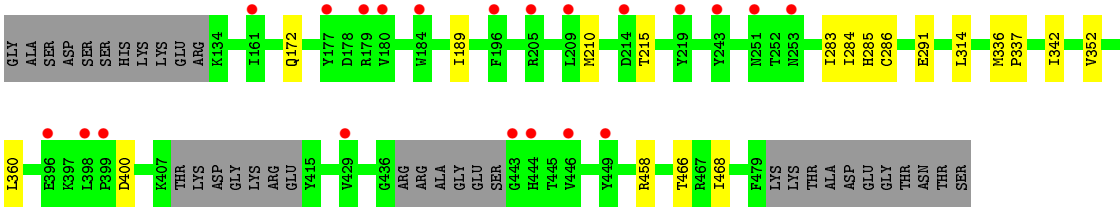


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	10	3	1	1		
2	B	1	Total	C	N	O	S	0	0
			15	10	3	1	1		
2	C	1	Total	C	N	O	S	0	0
			15	10	3	1	1		
2	D	1	Total	C	N	O	S	0	0
			15	10	3	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		
3	B	35	Total	O	0	0
			35	35		
3	C	36	Total	O	0	0
			36	36		
3	D	37	Total	O	0	0
			37	37		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.75Å 87.70Å 229.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.19 – 2.15 48.19 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.19-2.15) 98.7 (48.19-2.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.204 , 0.234 0.200 , 0.230	Depositor DCC
$R_{free}$ test set	5538 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 19.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.426 for k,h,-l	Xtriage
Reported twinning fraction	0.571 for H, K, L 0.429 for K, H, -L	Depositor
Outliers	0 of 110551 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11182	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.35	0/2842	0.53	0/3833
1	B	0.31	0/2808	0.51	0/3789
1	C	0.33	0/2724	0.52	0/3686
1	D	0.31	0/2758	0.50	0/3723
All	All	0.32	0/11132	0.51	0/15031

There are no bond length outliers.

There are no bond angle outliers.

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	2794	0	2787	8	0
1	B	2761	0	2745	8	0
1	C	2678	0	2599	8	0
1	D	2711	0	2693	9	0
2	A	15	0	0	1	0
2	B	15	0	0	1	0
2	C	15	0	0	1	0
2	D	15	0	0	1	0
3	A	70	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	35	0	0	0	0
3	C	36	0	0	0	0
3	D	37	0	0	0	0
All	All	11182	0	10824	34	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 2.

All (34) 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:D:458:ARG:NH2	1:D:466:THR:O	2.16	0.76
1:A:395:PHE:HB3	3:A:2053:HOH:O	1.88	0.72
2:B:1482:AJG:SAJ	2:B:1482:AJG:CAA	2.85	0.64
2:A:1482:AJG:SAJ	2:A:1482:AJG:CAA	2.88	0.62
2:C:1481:AJG:SAJ	2:C:1481:AJG:CAA	2.91	0.59
1:D:284:ILE:HG21	1:D:342:ILE:HD11	1.93	0.50
1:C:458:ARG:HG3	1:C:468:ILE:HB	1.93	0.49
1:D:352:VAL:HG11	1:D:360:LEU:HD13	1.94	0.49
1:C:322:ILE:O	1:C:328:ARG:NH1	2.46	0.48
1:D:210:MET:CE	1:D:283:ILE:HD13	2.45	0.46
2:D:1481:AJG:CAA	2:D:1481:AJG:SAJ	3.04	0.46
1:B:135:VAL:CG1	1:B:139:GLY:N	2.78	0.46
1:B:314:LEU:O	1:C:315:GLY:HA2	2.16	0.46
1:C:421:ARG:HG2	1:C:426:ILE:HD11	1.98	0.45
1:A:480:LYS:NZ	3:A:2069:HOH:O	2.49	0.45
1:A:396:GLU:N	3:A:2053:HOH:O	2.49	0.45
1:A:312:CYS:HB2	3:A:2034:HOH:O	2.17	0.45
1:C:155:TRP:HB2	1:C:159:TYR:HB2	1.99	0.45
1:A:315:GLY:HA2	1:D:314:LEU:O	2.18	0.43
1:A:279:PRO:HG3	1:D:337:PRO:HG3	2.01	0.43
1:B:135:VAL:HG13	1:B:139:GLY:HA2	1.99	0.43
1:D:172:GLN:O	1:D:189:ILE:N	2.48	0.43
1:D:285:HIS:O	1:D:286:CYS:HB2	2.18	0.42
1:C:321:PTR:O1P	1:C:328:ARG:NH2	2.52	0.42
1:B:249:LEU:HD22	1:B:357:GLY:HA2	2.01	0.42
1:B:361:PHE:CE1	1:B:373:ILE:HA	2.55	0.42
1:B:279:PRO:O	1:B:282:SER:OG	2.38	0.42
1:A:207:LEU:HA	1:A:210:MET:HE3	2.01	0.41
1:C:331:GLU:OE2	1:C:467:ARG:NH1	2.53	0.41
1:A:336:MET:HB3	1:A:337:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:ILE:O	1:D:468:ILE:HG23	2.21	0.41
1:B:159:TYR:OH	1:B:226:ARG:HD2	2.21	0.40
1:C:308:PHE:HD2	1:C:311:SER:HG	1.64	0.40
1:B:222:VAL:HB	1:B:306:VAL:HG12	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	337/368 (92%)	317 (94%)	20 (6%)	0	100	100
1	B	335/368 (91%)	312 (93%)	22 (7%)	1 (0%)	41	37
1	C	326/368 (89%)	308 (94%)	18 (6%)	0	100	100
1	D	326/368 (89%)	305 (94%)	21 (6%)	0	100	100
All	All	1324/1472 (90%)	1242 (94%)	81 (6%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	217	MET

### 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	301/324 (93%)	299 (99%)	2 (1%)	84	89
1	B	296/324 (91%)	292 (99%)	4 (1%)	67	72
1	C	282/324 (87%)	281 (100%)	1 (0%)	91	93
1	D	292/324 (90%)	288 (99%)	4 (1%)	67	72
All	All	1171/1296 (90%)	1160 (99%)	11 (1%)	78	83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	ASP
1	A	465	LYS
1	B	219	TYR
1	B	282	SER
1	B	404	ASN
1	B	465	LYS
1	C	194	LYS
1	D	215	THR
1	D	291	GLU
1	D	336	MET
1	D	400	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	251	ASN
1	A	383	HIS
1	A	469	GLN
1	B	260	ASN
1	D	383	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	D	321	1	15,16,17	0.69	0	19,22,24	0.76	0
1	PTR	A	321	1	15,16,17	0.77	0	19,22,24	0.87	0
1	PTR	C	321	1	15,16,17	0.95	1 (6%)	19,22,24	0.76	1 (5%)
1	PTR	B	321	1	15,16,17	0.81	0	19,22,24	0.88	0

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	D	321	1	-	2/10/11/13	0/1/1/1
1	PTR	A	321	1	-	0/10/11/13	0/1/1/1
1	PTR	C	321	1	-	0/10/11/13	0/1/1/1
1	PTR	B	321	1	-	0/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	321	PTR	P-OH	2.54	1.63	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	PTR	O3P-P-O2P	2.37	116.71	107.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	321	PTR	O-C-CA-CB
1	D	321	PTR	CZ-OH-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	321	PTR	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands 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
2	AJG	D	1481	-	14,16,16	4.46	4 (28%)	16,22,22	1.74	4 (25%)
2	AJG	C	1481	-	14,16,16	3.73	4 (28%)	16,22,22	1.90	5 (31%)
2	AJG	A	1482	-	14,16,16	5.80	4 (28%)	16,22,22	1.83	5 (31%)
2	AJG	B	1482	-	14,16,16	6.24	4 (28%)	16,22,22	1.87	5 (31%)

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
2	AJG	D	1481	-	-	2/4/6/6	0/2/2/2
2	AJG	C	1481	-	-	2/4/6/6	0/2/2/2
2	AJG	A	1482	-	-	2/4/6/6	0/2/2/2
2	AJG	B	1482	-	-	2/4/6/6	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1482	AJG	CAO-SAJ	-22.46	1.56	1.74
2	A	1482	AJG	CAO-SAJ	-20.72	1.58	1.74
2	D	1481	AJG	CAO-SAJ	-15.46	1.62	1.74
2	C	1481	AJG	CAO-SAJ	-12.38	1.64	1.74
2	C	1481	AJG	CAF-CAN	-4.69	1.33	1.41
2	B	1482	AJG	CAF-CAN	-4.56	1.33	1.41
2	A	1482	AJG	CAF-CAN	-4.44	1.34	1.41
2	D	1481	AJG	CAF-CAN	-4.39	1.34	1.41
2	B	1482	AJG	CAA-CAK	2.81	1.53	1.49
2	A	1482	AJG	CAA-CAK	2.69	1.53	1.49
2	C	1481	AJG	CAA-CAK	2.58	1.53	1.49
2	D	1481	AJG	CAA-CAK	2.51	1.53	1.49
2	B	1482	AJG	CAN-CAO	-2.15	1.35	1.42
2	C	1481	AJG	CAN-CAO	-2.13	1.35	1.42
2	A	1482	AJG	CAG-CAO	-2.13	1.33	1.38
2	D	1481	AJG	CAN-CAO	-2.06	1.35	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1481	AJG	CAA-CAK-NAI	3.92	120.92	114.85
2	B	1482	AJG	CAA-CAK-NAI	3.90	120.90	114.85
2	A	1482	AJG	CAA-CAK-NAI	3.78	120.71	114.85
2	C	1481	AJG	CAM-NAI-CAK	3.72	125.77	116.11
2	A	1482	AJG	CAM-NAI-CAK	3.50	125.21	116.11
2	B	1482	AJG	CAM-NAI-CAK	3.46	125.11	116.11
2	D	1481	AJG	CAM-NAI-CAK	3.28	124.64	116.11
2	D	1481	AJG	CAA-CAK-NAI	3.23	119.86	114.85
2	B	1482	AJG	CAN-CAO-SAJ	-3.08	107.77	111.85
2	D	1481	AJG	CAN-CAO-SAJ	-2.97	107.91	111.85
2	C	1481	AJG	CAN-CAO-SAJ	-2.84	108.09	111.85
2	A	1482	AJG	CAN-CAO-SAJ	-2.74	108.21	111.85
2	D	1481	AJG	CAG-CAO-SAJ	2.41	129.92	125.10
2	C	1481	AJG	CAG-CAO-SAJ	2.26	129.63	125.10
2	A	1482	AJG	CAO-CAN-NAH	2.25	113.27	108.04
2	C	1481	AJG	CAO-CAN-NAH	2.20	113.17	108.04
2	B	1482	AJG	CAG-CAO-SAJ	2.17	129.44	125.10
2	A	1482	AJG	CAG-CAO-SAJ	2.11	129.32	125.10
2	B	1482	AJG	CAO-CAN-NAH	2.07	112.85	108.04

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1481	AJG	OAC-CAK-NAI-CAM
2	D	1481	AJG	CAA-CAK-NAI-CAM
2	C	1481	AJG	OAC-CAK-NAI-CAM
2	C	1481	AJG	CAA-CAK-NAI-CAM
2	A	1482	AJG	OAC-CAK-NAI-CAM
2	A	1482	AJG	CAA-CAK-NAI-CAM
2	B	1482	AJG	OAC-CAK-NAI-CAM
2	B	1482	AJG	CAA-CAK-NAI-CAM

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1481	AJG	1	0
2	C	1481	AJG	1	0
2	A	1482	AJG	1	0
2	B	1482	AJG	1	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<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	341/368 (92%)	0.46	6 (1%) 68 75	23, 36, 56, 68	0
1	B	339/368 (92%)	0.77	21 (6%) 20 27	27, 47, 76, 91	0
1	C	332/368 (90%)	0.75	23 (6%) 16 23	25, 47, 68, 80	0
1	D	332/368 (90%)	0.69	21 (6%) 20 27	25, 47, 72, 89	0
All	All	1344/1472 (91%)	0.67	71 (5%) 26 35	23, 44, 69, 91	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	423	LEU	4.7
1	C	472	TYR	4.7
1	D	446	VAL	4.4
1	C	384	ILE	4.3
1	B	243	TYR	4.0
1	B	402	THR	3.9
1	B	449	TYR	3.8
1	D	219	TYR	3.8
1	D	184	TRP	3.8
1	B	398	LEU	3.6
1	B	384	ILE	3.6
1	C	136	TYR	3.5
1	B	215	THR	3.5
1	D	399	PRO	3.4
1	C	312	CYS	3.4
1	D	253	ASN	3.3
1	D	443	GLY	3.3
1	D	398	LEU	3.2
1	A	214	ASP	3.2
1	C	457	LEU	3.1
1	B	216	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	395	PHE	2.8
1	C	440	GLY	2.8
1	A	219	TYR	2.7
1	C	378	GLY	2.7
1	C	424	HIS	2.7
1	D	205	ARG	2.7
1	C	334	LEU	2.7
1	B	217	MET	2.6
1	A	140	TYR	2.5
1	D	180	VAL	2.5
1	B	374	VAL	2.5
1	D	243	TYR	2.5
1	C	427	LEU	2.4
1	D	444	HIS	2.4
1	C	245	LEU	2.4
1	C	456	ILE	2.4
1	D	449	TYR	2.4
1	B	394	PHE	2.4
1	B	401	GLY	2.4
1	C	450	LEU	2.4
1	D	161	ILE	2.4
1	D	177	TYR	2.4
1	B	133	ARG	2.4
1	C	478	PHE	2.4
1	D	251	ASN	2.4
1	D	196	PHE	2.3
1	B	270	CYS	2.3
1	B	333	LEU	2.3
1	A	136	TYR	2.3
1	A	318	ILE	2.3
1	C	135	VAL	2.3
1	C	455	LEU	2.2
1	C	379	ILE	2.2
1	D	396	GLU	2.2
1	D	429	VAL	2.2
1	D	214	ASP	2.2
1	C	429	VAL	2.1
1	C	270	CYS	2.1
1	D	179	ARG	2.1
1	B	396	GLU	2.1
1	B	399	PRO	2.1
1	B	474	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	243	TYR	2.1
1	D	209	LEU	2.1
1	C	341	ALA	2.1
1	B	376	VAL	2.0
1	B	425	ASN	2.0
1	B	220	TYR	2.0
1	C	471	TYR	2.0
1	B	460	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PTR	C	321	16/17	0.87	0.16	37,41,43,44	0
1	PTR	D	321	16/17	0.91	0.15	32,35,43,45	0
1	PTR	B	321	16/17	0.93	0.13	42,46,49,49	0
1	PTR	A	321	16/17	0.94	0.15	27,30,35,36	0

## 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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	AJG	D	1481	15/15	0.84	0.20	52,57,64,64	0
2	AJG	B	1482	15/15	0.92	0.18	46,49,59,63	0
2	AJG	C	1481	15/15	0.93	0.13	37,40,42,45	0
2	AJG	A	1482	15/15	0.94	0.12	39,40,45,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.