



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:14 PM UTC

PDB ID : 5A4E / pdb\_00005a4e  
Title : DYRK1A in complex with methoxy benzothiazole fragment  
Authors : Rothweiler, U.  
Deposited on : 2015-06-08  
Resolution : 2.68 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
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

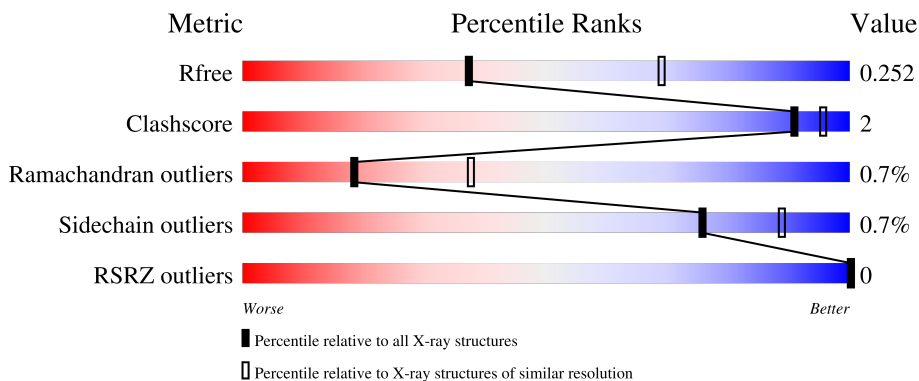
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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  $\geq 3$ , 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	
1	B	368	
1	C	368	
1	D	368	

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
2	7QQ	A	1482[B]	-	X	-	-
2	7QQ	B	1482[B]	-	X	-	-
2	7QQ	C	1475[A]	-	X	-	-
2	7QQ	C	1475[B]	-	X	-	-
2	7QQ	D	1482[B]	-	X	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10499 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.

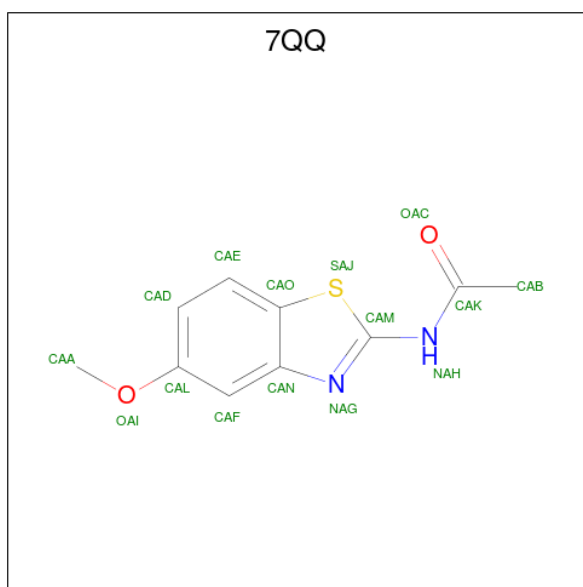
- Molecule 1 is a protein called DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	342	Total 2792	C 1798	N 475	O 501	P 1	S 17	0	0	0
1	B	323	Total 2630	C 1697	N 448	O 468	P 1	S 16	0	0	0
1	C	263	Total 2161	C 1390	N 367	O 386	P 1	S 17	0	0	0
1	D	332	Total 2706	C 1750	N 453	O 485	P 1	S 17	0	0	0

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-(5-methoxy-1,3-benzothiazol-2-yl)ethanamide (CCD ID: 7QQ) (formula: C<sub>10</sub>H<sub>10</sub>N<sub>2</sub>O<sub>2</sub>S).

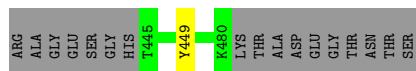


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			30	20	4	4	2		
2	B	1	Total	C	N	O	S	0	1
			30	20	4	4	2		
2	C	1	Total	C	N	O	S	0	1
			30	20	4	4	2		
2	D	1	Total	C	N	O	S	0	1
			30	20	4	4	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	15	Total	O	0	0
			15	15		
3	C	9	Total	O	0	0
			9	9		
3	D	22	Total	O	0	0
			22	22		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.08Å 87.10Å 226.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.54 – 2.68 47.54 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.54-2.68) 97.3 (47.54-2.68)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.79 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.236 , 0.268 0.226 , 0.252	Depositor DCC
$R_{free}$ test set	2101 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.0	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 15.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.309 for k,h,-l	Xtriage
Reported twinning fraction	0.702 for H, K, L 0.298 for K, H, -L	Depositor
Outliers	0 of 48635 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10499	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: 7QQ, PTR

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	0.40	0/2840	0.64	0/3830
1	B	0.40	0/2673	0.65	0/3604
1	C	0.37	0/2188	0.64	0/2947
1	D	0.38	0/2752	0.64	0/3714
All	All	0.39	0/10453	0.64	0/14095

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	2792	0	2785	6	0
1	B	2630	0	2623	4	0
1	C	2161	0	2150	6	0
1	D	2706	0	2696	10	0
2	A	30	0	0	2	0
2	B	30	0	0	2	0
2	C	30	0	0	2	0
2	D	30	0	0	2	0
3	A	44	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	0	0
3	C	9	0	0	0	0
3	D	22	0	0	0	0
All	All	10499	0	10254	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)
2:D:1482[A]:7QQ:SAJ	2:D:1482[A]:7QQ:CAB	2.19	1.29
2:A:1482[B]:7QQ:CAB	2:A:1482[B]:7QQ:NAG	2.21	1.01
2:B:1482[B]:7QQ:NAG	2:B:1482[B]:7QQ:CAB	2.24	0.99
2:C:1475[B]:7QQ:CAB	2:C:1475[B]:7QQ:NAG	2.23	0.95
2:D:1482[B]:7QQ:CAB	2:D:1482[B]:7QQ:NAG	2.27	0.94
2:C:1475[A]:7QQ:CAB	2:C:1475[A]:7QQ:NAG	2.29	0.90
2:A:1482[A]:7QQ:CAB	2:A:1482[A]:7QQ:NAG	2.47	0.77
2:B:1482[A]:7QQ:OAC	2:B:1482[A]:7QQ:SAJ	2.53	0.66
1:C:257:VAL:HG11	1:C:261:LEU:HD23	1.82	0.61
1:B:293:ILE:CG2	1:B:303:ILE:HD11	2.33	0.58
1:B:293:ILE:HG21	1:B:303:ILE:HD11	1.89	0.55
1:C:210:MET:CE	1:C:221:ILE:HD13	2.36	0.55
1:D:176:ALA:HB3	1:D:187:ILE:HD13	1.90	0.54
1:C:248:LEU:HD11	1:C:295:LEU:HD11	1.90	0.53
1:D:210:MET:HE1	1:D:308:PHE:CE2	2.45	0.52
1:A:370:MET:O	1:A:374:VAL:HG23	2.12	0.50
1:A:161:ILE:HG23	1:A:174:VAL:HG21	1.96	0.47
1:D:147:TYR:O	1:D:172:GLN:NE2	2.48	0.47
1:C:210:MET:HE2	1:C:221:ILE:HD13	1.96	0.47
1:A:352:VAL:HG11	1:A:360:LEU:HD13	1.98	0.46
1:D:187:ILE:HD12	1:D:187:ILE:N	2.31	0.45
1:C:257:VAL:HG11	1:C:261:LEU:CD2	2.46	0.45
1:B:265:PHE:CD1	1:B:303:ILE:HD12	2.52	0.45
1:D:294:LEU:HD13	1:D:306:VAL:HG21	1.99	0.45
1:A:216:GLU:O	1:A:218:LYS:N	2.51	0.44
1:D:324:SER:O	1:D:325:ARG:C	2.61	0.44
1:D:165:ILE:HD13	1:D:240:MET:HE1	2.00	0.43
1:D:429:VAL:HG22	1:D:449:TYR:HB3	2.00	0.43
1:A:249:LEU:HD21	1:A:353:GLU:HG2	2.00	0.42
1:B:289:LYS:HB2	1:B:290:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:VAL:HG23	1:D:187:ILE:HD11	2.02	0.41
1:D:388:ALA:HB3	1:D:391:ALA:HB2	2.02	0.41
1:C:269:MET:SD	1:C:305:ILE:HD11	2.61	0.40
1:A:374:VAL:HG11	1:A:405:LEU:HD11	2.03	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%)	318 (94%)	15 (4%)	4 (1%)	10	24
1	B	316/368 (86%)	299 (95%)	16 (5%)	1 (0%)	36	57
1	C	254/368 (69%)	234 (92%)	17 (7%)	3 (1%)	10	24
1	D	325/368 (88%)	304 (94%)	20 (6%)	1 (0%)	36	57
All	All	1232/1472 (84%)	1155 (94%)	68 (6%)	9 (1%)	18	37

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	MET
1	A	215	THR
1	C	287	ASP
1	A	287	ASP
1	A	307	ASP
1	B	323	GLN
1	C	242	SER
1	C	298	PRO
1	D	434	PRO

### 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%)	76	89
1	B	282/324 (87%)	280 (99%)	2 (1%)	76	89
1	C	233/324 (72%)	230 (99%)	3 (1%)	61	81
1	D	292/324 (90%)	291 (100%)	1 (0%)	86	94
All	All	1108/1296 (86%)	1100 (99%)	8 (1%)	76	89

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	SER
1	A	310	SER
1	B	197	LEU
1	B	286	CYS
1	C	286	CYS
1	C	306	VAL
1	C	336	MET
1	D	385	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	213	HIS
1	A	425	ASN
1	A	475	GLN
1	B	198	ASN
1	B	201	GLN
1	B	223	HIS
1	B	313	GLN
1	B	383	HIS
1	B	476	HIS
1	C	199	GLN

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Mol	Chain	Res	Type
1	C	253	ASN
1	D	137	ASN
1	D	172	GLN
1	D	192	ASN
1	D	223	HIS
1	D	232	ASN
1	D	267	GLN
1	D	313	GLN
1	D	476	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PTR	B	321	1	15,16,17	0.68	0	17,22,24	0.83	0
1	PTR	A	321	1	15,16,17	0.71	0	17,22,24	0.83	0
1	PTR	D	321	1	15,16,17	0.69	0	17,22,24	0.82	0
1	PTR	C	321	1	15,16,17	0.70	0	17,22,24	0.82	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	B	321	1	-	0/10/11/13	0/1/1/1
1	PTR	A	321	1	-	0/10/11/13	0/1/1/1
1	PTR	D	321	1	-	1/10/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	C	321	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	321	PTR	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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	7QQ	D	1482[B]	-	16,16,16	3.82	7 (43%)	22,22,22	2.79	6 (27%)
2	7QQ	D	1482[A]	-	16,16,16	3.89	7 (43%)	22,22,22	2.83	6 (27%)
2	7QQ	A	1482[B]	-	16,16,16	3.69	7 (43%)	22,22,22	2.75	7 (31%)
2	7QQ	A	1482[A]	-	16,16,16	4.35	7 (43%)	22,22,22	2.94	6 (27%)
2	7QQ	C	1475[A]	-	16,16,16	4.43	7 (43%)	22,22,22	2.92	6 (27%)
2	7QQ	B	1482[B]	-	16,16,16	4.12	7 (43%)	22,22,22	2.81	6 (27%)
2	7QQ	B	1482[A]	-	16,16,16	4.12	7 (43%)	22,22,22	2.84	7 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	7QQ	C	1475[B]	-	16,16,16	4.02	7 (43%)	22,22,22	2.82	7 (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	7QQ	D	1482[B]	-	-	6/6/6/6	0/2/2/2
2	7QQ	D	1482[A]	-	-	2/6/6/6	0/2/2/2
2	7QQ	A	1482[B]	-	-	6/6/6/6	0/2/2/2
2	7QQ	A	1482[A]	-	-	4/6/6/6	0/2/2/2
2	7QQ	C	1475[A]	-	-	6/6/6/6	0/2/2/2
2	7QQ	B	1482[B]	-	-	6/6/6/6	0/2/2/2
2	7QQ	B	1482[A]	-	-	2/6/6/6	0/2/2/2
2	7QQ	C	1475[B]	-	-	6/6/6/6	0/2/2/2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1475[A]	7QQ	CAM-SAJ	-14.89	1.57	1.75
2	A	1482[A]	7QQ	CAM-SAJ	-14.60	1.57	1.75
2	B	1482[B]	7QQ	CAM-SAJ	-13.57	1.59	1.75
2	B	1482[A]	7QQ	CAM-SAJ	-13.43	1.59	1.75
2	C	1475[B]	7QQ	CAM-SAJ	-13.10	1.59	1.75
2	D	1482[A]	7QQ	CAM-SAJ	-12.46	1.60	1.75
2	D	1482[B]	7QQ	CAM-SAJ	-12.34	1.60	1.75
2	A	1482[B]	7QQ	CAM-SAJ	-11.83	1.61	1.75
2	A	1482[A]	7QQ	CAO-SAJ	-5.58	1.63	1.74
2	C	1475[A]	7QQ	CAO-SAJ	-5.44	1.63	1.74
2	B	1482[A]	7QQ	CAO-SAJ	-5.12	1.64	1.74
2	D	1482[A]	7QQ	CAO-SAJ	-5.07	1.64	1.74
2	B	1482[B]	7QQ	CAO-SAJ	-4.88	1.64	1.74
2	C	1475[B]	7QQ	CAO-SAJ	-4.60	1.65	1.74
2	D	1482[B]	7QQ	CAO-SAJ	-4.35	1.65	1.74
2	C	1475[B]	7QQ	CAF-CAN	-4.21	1.33	1.40
2	B	1482[A]	7QQ	CAF-CAN	-4.11	1.33	1.40
2	A	1482[B]	7QQ	CAF-CAN	-4.08	1.33	1.40
2	A	1482[B]	7QQ	CAO-SAJ	-4.06	1.66	1.74
2	B	1482[B]	7QQ	CAF-CAN	-4.06	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1482[A]	7QQ	CAF-CAN	-4.05	1.33	1.40
2	D	1482[B]	7QQ	CAF-CAN	-4.03	1.33	1.40
2	C	1475[A]	7QQ	CAF-CAN	-3.93	1.34	1.40
2	B	1482[A]	7QQ	CAE-CAO	-3.85	1.33	1.39
2	C	1475[A]	7QQ	CAE-CAO	-3.83	1.33	1.39
2	B	1482[B]	7QQ	CAE-CAO	-3.77	1.33	1.39
2	C	1475[B]	7QQ	CAE-CAO	-3.75	1.33	1.39
2	A	1482[A]	7QQ	CAE-CAO	-3.74	1.33	1.39
2	D	1482[A]	7QQ	CAE-CAO	-3.70	1.33	1.39
2	A	1482[A]	7QQ	CAF-CAN	-3.69	1.34	1.40
2	D	1482[B]	7QQ	CAE-CAO	-3.67	1.33	1.39
2	A	1482[B]	7QQ	CAE-CAO	-3.67	1.33	1.39
2	B	1482[B]	7QQ	CAM-NAH	-3.44	1.33	1.38
2	C	1475[A]	7QQ	CAM-NAH	-3.39	1.33	1.38
2	C	1475[B]	7QQ	CAM-NAH	-3.36	1.33	1.38
2	B	1482[B]	7QQ	CAN-CAO	-3.30	1.35	1.40
2	B	1482[A]	7QQ	CAM-NAH	-3.30	1.33	1.38
2	C	1475[B]	7QQ	CAN-CAO	-3.29	1.35	1.40
2	C	1475[A]	7QQ	CAN-CAO	-3.27	1.35	1.40
2	D	1482[B]	7QQ	CAN-CAO	-3.27	1.35	1.40
2	D	1482[B]	7QQ	CAM-NAH	-3.25	1.33	1.38
2	D	1482[A]	7QQ	CAN-CAO	-3.23	1.35	1.40
2	B	1482[A]	7QQ	CAN-CAO	-3.20	1.35	1.40
2	A	1482[B]	7QQ	CAN-CAO	-3.18	1.35	1.40
2	A	1482[B]	7QQ	CAM-NAH	-3.18	1.33	1.38
2	D	1482[A]	7QQ	CAM-NAH	-3.18	1.33	1.38
2	A	1482[A]	7QQ	CAN-CAO	-3.16	1.35	1.40
2	A	1482[A]	7QQ	CAM-NAH	-3.11	1.33	1.38
2	B	1482[A]	7QQ	CAN-NAG	-2.36	1.35	1.39
2	C	1475[B]	7QQ	CAN-NAG	-2.30	1.35	1.39
2	D	1482[A]	7QQ	CAN-NAG	-2.27	1.35	1.39
2	D	1482[B]	7QQ	CAN-NAG	-2.27	1.35	1.39
2	A	1482[B]	7QQ	CAN-NAG	-2.24	1.35	1.39
2	B	1482[B]	7QQ	CAN-NAG	-2.18	1.35	1.39
2	C	1475[A]	7QQ	CAN-NAG	-2.15	1.35	1.39
2	A	1482[A]	7QQ	CAN-NAG	-2.06	1.35	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1482[A]	7QQ	CAO-SAJ-CAM	9.42	97.05	88.33
2	C	1475[A]	7QQ	CAO-SAJ-CAM	9.29	96.93	88.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1482[B]	7QQ	CAO-SAJ-CAM	8.58	96.27	88.33
2	B	1482[A]	7QQ	CAO-SAJ-CAM	8.54	96.23	88.33
2	D	1482[A]	7QQ	CAO-SAJ-CAM	8.43	96.13	88.33
2	C	1475[B]	7QQ	CAO-SAJ-CAM	8.38	96.08	88.33
2	D	1482[B]	7QQ	CAO-SAJ-CAM	8.14	95.87	88.33
2	A	1482[B]	7QQ	CAO-SAJ-CAM	7.90	95.64	88.33
2	A	1482[A]	7QQ	SAJ-CAM-NAG	-6.50	109.25	117.06
2	D	1482[A]	7QQ	SAJ-CAM-NAG	-6.49	109.26	117.06
2	D	1482[B]	7QQ	SAJ-CAM-NAG	-6.39	109.38	117.06
2	A	1482[B]	7QQ	SAJ-CAM-NAG	-6.34	109.44	117.06
2	C	1475[A]	7QQ	SAJ-CAM-NAG	-6.30	109.49	117.06
2	B	1482[A]	7QQ	SAJ-CAM-NAG	-6.28	109.51	117.06
2	C	1475[B]	7QQ	SAJ-CAM-NAG	-6.25	109.55	117.06
2	B	1482[B]	7QQ	SAJ-CAM-NAG	-6.17	109.64	117.06
2	C	1475[B]	7QQ	CAK-NAH-CAM	-4.90	115.98	124.05
2	D	1482[A]	7QQ	CAK-NAH-CAM	-4.65	116.39	124.05
2	A	1482[B]	7QQ	CAK-NAH-CAM	-4.60	116.48	124.05
2	B	1482[B]	7QQ	CAK-NAH-CAM	-4.33	116.92	124.05
2	D	1482[B]	7QQ	CAK-NAH-CAM	-4.30	116.97	124.05
2	A	1482[A]	7QQ	CAK-NAH-CAM	-4.25	117.06	124.05
2	B	1482[A]	7QQ	CAA-OAI-CAL	-4.16	108.59	117.50
2	B	1482[A]	7QQ	CAK-NAH-CAM	-4.15	117.23	124.05
2	C	1475[A]	7QQ	CAK-NAH-CAM	-3.92	117.60	124.05
2	D	1482[B]	7QQ	CAA-OAI-CAL	-3.77	109.41	117.50
2	C	1475[A]	7QQ	CAA-OAI-CAL	-3.73	109.49	117.50
2	B	1482[B]	7QQ	CAA-OAI-CAL	-3.43	110.14	117.50
2	A	1482[A]	7QQ	NAH-CAM-NAG	3.41	126.69	120.87
2	C	1475[B]	7QQ	CAA-OAI-CAL	-3.39	110.23	117.50
2	C	1475[A]	7QQ	NAH-CAM-NAG	3.36	126.61	120.87
2	A	1482[B]	7QQ	CAA-OAI-CAL	-3.28	110.46	117.50
2	D	1482[A]	7QQ	CAA-OAI-CAL	-3.21	110.61	117.50
2	B	1482[B]	7QQ	NAH-CAM-NAG	2.87	125.78	120.87
2	D	1482[B]	7QQ	NAH-CAM-NAG	2.75	125.56	120.87
2	A	1482[A]	7QQ	CAA-OAI-CAL	-2.72	111.66	117.50
2	D	1482[A]	7QQ	NAH-CAM-NAG	2.71	125.50	120.87
2	A	1482[B]	7QQ	NAH-CAM-NAG	2.52	125.17	120.87
2	B	1482[A]	7QQ	NAH-CAM-NAG	2.39	124.95	120.87
2	A	1482[B]	7QQ	CAN-NAG-CAM	2.32	114.17	108.66
2	D	1482[B]	7QQ	CAN-NAG-CAM	2.30	114.12	108.66
2	C	1475[B]	7QQ	NAH-CAM-NAG	2.26	124.72	120.87
2	D	1482[A]	7QQ	CAN-NAG-CAM	2.21	113.90	108.66
2	C	1475[B]	7QQ	SAJ-CAM-NAH	2.20	125.72	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1475[B]	7QQ	CAN-NAG-CAM	2.20	113.86	108.66
2	B	1482[A]	7QQ	CAN-NAG-CAM	2.16	113.78	108.66
2	A	1482[A]	7QQ	CAN-NAG-CAM	2.14	113.72	108.66
2	B	1482[B]	7QQ	CAN-NAG-CAM	2.11	113.66	108.66
2	B	1482[A]	7QQ	SAJ-CAM-NAH	2.09	125.53	121.87
2	C	1475[A]	7QQ	CAN-NAG-CAM	2.08	113.60	108.66
2	A	1482[B]	7QQ	SAJ-CAM-NAH	2.01	125.39	121.87

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1482[A]	7QQ	CAB-CAK-NAH-CAM
2	A	1482[A]	7QQ	OAC-CAK-NAH-CAM
2	A	1482[A]	7QQ	SAJ-CAM-NAH-CAK
2	A	1482[A]	7QQ	NAG-CAM-NAH-CAK
2	A	1482[B]	7QQ	CAB-CAK-NAH-CAM
2	A	1482[B]	7QQ	OAC-CAK-NAH-CAM
2	A	1482[B]	7QQ	SAJ-CAM-NAH-CAK
2	A	1482[B]	7QQ	NAG-CAM-NAH-CAK
2	B	1482[B]	7QQ	CAB-CAK-NAH-CAM
2	B	1482[B]	7QQ	OAC-CAK-NAH-CAM
2	B	1482[B]	7QQ	SAJ-CAM-NAH-CAK
2	B	1482[B]	7QQ	NAG-CAM-NAH-CAK
2	C	1475[A]	7QQ	CAB-CAK-NAH-CAM
2	C	1475[A]	7QQ	OAC-CAK-NAH-CAM
2	C	1475[A]	7QQ	SAJ-CAM-NAH-CAK
2	C	1475[A]	7QQ	NAG-CAM-NAH-CAK
2	C	1475[B]	7QQ	CAB-CAK-NAH-CAM
2	C	1475[B]	7QQ	OAC-CAK-NAH-CAM
2	C	1475[B]	7QQ	SAJ-CAM-NAH-CAK
2	C	1475[B]	7QQ	NAG-CAM-NAH-CAK
2	D	1482[A]	7QQ	CAB-CAK-NAH-CAM
2	D	1482[A]	7QQ	OAC-CAK-NAH-CAM
2	D	1482[B]	7QQ	CAB-CAK-NAH-CAM
2	D	1482[B]	7QQ	OAC-CAK-NAH-CAM
2	D	1482[B]	7QQ	SAJ-CAM-NAH-CAK
2	D	1482[B]	7QQ	NAG-CAM-NAH-CAK
2	A	1482[B]	7QQ	CAF-CAL-OAI-CAA
2	B	1482[B]	7QQ	CAF-CAL-OAI-CAA
2	A	1482[B]	7QQ	CAD-CAL-OAI-CAA
2	B	1482[B]	7QQ	CAD-CAL-OAI-CAA

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Mol	Chain	Res	Type	Atoms
2	C	1475[A]	7QQ	CAF-CAL-OAI-CAA
2	C	1475[A]	7QQ	CAD-CAL-OAI-CAA
2	C	1475[B]	7QQ	CAD-CAL-OAI-CAA
2	C	1475[B]	7QQ	CAF-CAL-OAI-CAA
2	D	1482[B]	7QQ	CAF-CAL-OAI-CAA
2	D	1482[B]	7QQ	CAD-CAL-OAI-CAA
2	B	1482[A]	7QQ	CAD-CAL-OAI-CAA
2	B	1482[A]	7QQ	CAF-CAL-OAI-CAA

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1482[B]	7QQ	1	0
2	D	1482[A]	7QQ	1	0
2	A	1482[B]	7QQ	1	0
2	A	1482[A]	7QQ	1	0
2	C	1475[A]	7QQ	1	0
2	B	1482[B]	7QQ	1	0
2	B	1482[A]	7QQ	1	0
2	C	1475[B]	7QQ	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-1.21	0 100 100	32, 45, 66, 76	0
1	B	322/368 (87%)	-1.06	0 100 100	36, 60, 82, 94	0
1	C	262/368 (71%)	-1.06	0 100 100	44, 66, 88, 92	0
1	D	331/368 (89%)	-1.14	0 100 100	39, 58, 85, 95	0
All	All	1256/1472 (85%)	-1.12	0 100 100	32, 56, 85, 95	0

There are no RSRZ outliers to report.

### 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	A	321	16/17	0.99	0.05	43,44,45,47	0
1	PTR	B	321	16/17	0.99	0.04	58,60,61,61	0
1	PTR	C	321	16/17	0.99	0.05	63,64,64,65	0
1	PTR	D	321	16/17	0.99	0.04	46,47,48,48	0

### 6.3 Carbohydrates [i](#)

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, 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( $\text{\AA}^2$ )	Q<0.9
2	7QQ	C	1475[A]	15/15	0.98	0.07	58,59,60,60	15
2	7QQ	C	1475[B]	15/15	0.98	0.07	64,65,66,66	15
2	7QQ	B	1482[A]	15/15	0.99	0.06	46,47,48,48	15
2	7QQ	B	1482[B]	15/15	0.99	0.06	56,57,58,58	15
2	7QQ	A	1482[A]	15/15	0.99	0.06	42,42,43,43	15
2	7QQ	A	1482[B]	15/15	0.99	0.06	65,65,65,66	15
2	7QQ	D	1482[A]	15/15	0.99	0.04	43,43,45,45	15
2	7QQ	D	1482[B]	15/15	0.99	0.04	61,62,62,62	15

## 6.5 Other polymers [i](#)

There are no such residues in this entry.