



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:45 am GMT

PDB ID : 5A4E
Title : DYRK1A IN COMPLEX WITH METHOXY BENZOTHAZOL FRAGMENT
Authors : Rothweiler, U.
Deposited on : 2015-06-08
Resolution : 2.68 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

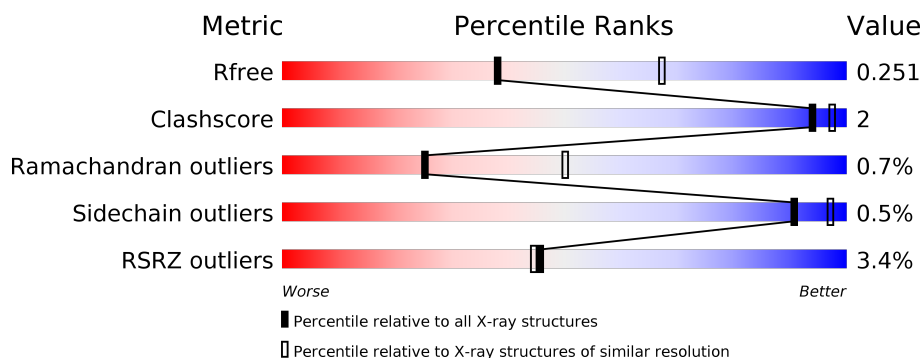
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	3050 (2.70-2.66)
Clashscore	112137	3418 (2.70-2.66)
Ramachandran outliers	110173	3367 (2.70-2.66)
Sidechain outliers	110143	3367 (2.70-2.66)
RSRZ outliers	101464	3069 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>88%</div> <div>5% 7%</div> </div>
1	B	368	<div> <div>4%</div> <div>86%</div> <div>12%</div> </div>
1	C	368	<div> <div>4%</div> <div>68%</div> <div>29%</div> </div>
1	D	368	<div> <div>3%</div> <div>86%</div> <div>10%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	7QQ	A	1482[A]	-	-	-	X
2	7QQ	A	1482[B]	-	-	-	X
2	7QQ	B	1482[A]	-	-	-	X
2	7QQ	B	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.

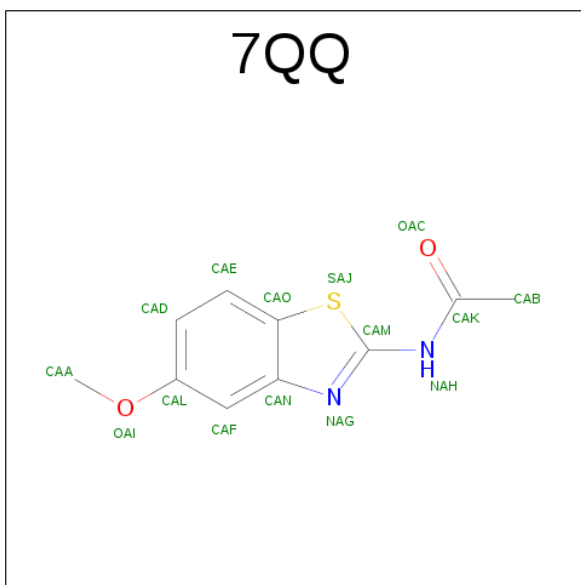
- Molecule 1 is a protein called DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	P	S	0	0	0
			2792	1798	475	501	1	17			
1	B	323	Total	C	N	O	P	S	0	0	0
			2630	1697	448	468	1	16			
1	C	263	Total	C	N	O	P	S	0	0	0
			2161	1390	367	386	1	17			
1	D	332	Total	C	N	O	P	S	0	0	0
			2706	1750	453	485	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-(5-METHOXY-1,3-BENZOTHAZOL-2-YL)ETHANAMIDE (three-letter code: 7QQ) (formula: C₁₀H₁₀N₂O₂S).



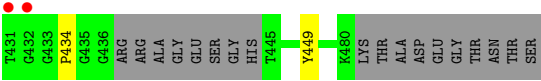
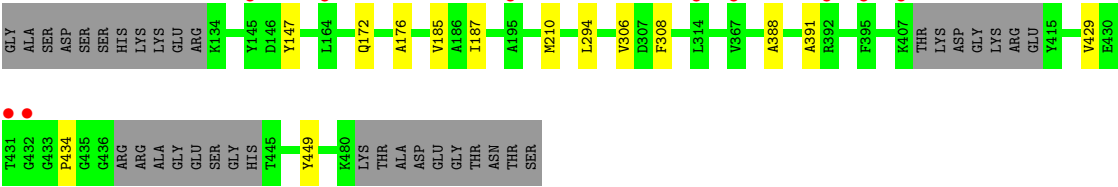
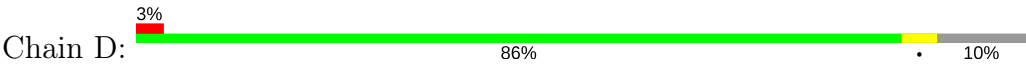
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			30	20	4	4	2		
2	B	1	Total	C	N	O	S	0	1
			30	20	4	4	2		
2	C	1	Total	C	N	O	S	0	1
			30	20	4	4	2		
2	D	1	Total	C	N	O	S	0	1
			30	20	4	4	2		

- 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		

- Molecule 1: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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) 97.1 (47.54-2.68)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.236 , 0.268 0.227 , 0.251	Depositor DCC
R_{free} test set	2072 reflections (4.52%)	DCC
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 13.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.308 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	0.90	EDS
Total number of atoms	10499	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, 7QQ

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	0.28	0/2840	0.46	0/3830
1	B	0.27	0/2673	0.44	0/3604
1	C	0.27	0/2188	0.45	0/2947
1	D	0.27	0/2752	0.44	0/3714
All	All	0.27	0/10453	0.45	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	8	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	32	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.

The worst 5 of 32 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:CAB	2:D:1482[A]:7QQ:SAJ	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:CAB	2:B:1482[B]:7QQ:NAG	2.24	0.99
2:C:1475[B]:7QQ:NAG	2:C:1475[B]:7QQ:CAB	2.23	0.95
2:D:1482[B]:7QQ:NAG	2:D:1482[B]:7QQ:CAB	2.27	0.94

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%)	15	34
1	B	316/368 (86%)	299 (95%)	16 (5%)	1 (0%)	44	71
1	C	254/368 (69%)	234 (92%)	17 (7%)	3 (1%)	15	34
1	D	325/368 (88%)	304 (94%)	20 (6%)	1 (0%)	44	71
All	All	1232/1472 (84%)	1155 (94%)	68 (6%)	9 (1%)	25	50

5 of 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

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	301/324 (93%)	299 (99%)	2 (1%)	87	95
1	B	282/324 (87%)	280 (99%)	2 (1%)	87	95
1	C	233/324 (72%)	231 (99%)	2 (1%)	82	94
1	D	292/324 (90%)	292 (100%)	0	100	100
All	All	1108/1296 (86%)	1102 (100%)	6 (0%)	91	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	197	LEU
1	C	286	CYS
1	B	286	CYS
1	A	310	SER
1	C	179	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	383	HIS
1	C	253	ASN
1	D	313	GLN

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	A	321	1	15,16,17	0.63	0	19,22,24	0.80	0
1	PTR	B	321	1	15,16,17	0.62	0	19,22,24	0.83	0
1	PTR	C	321	1	15,16,17	0.66	0	19,22,24	0.79	0
1	PTR	D	321	1	15,16,17	0.61	0	19,22,24	0.80	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	A	321	1	-	0/9/11/13	0/1/1/1
1	PTR	B	321	1	-	0/9/11/13	0/1/1/1
1	PTR	C	321	1	-	0/9/11/13	0/1/1/1
1	PTR	D	321	1	-	0/9/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	A	1482[A]	-	13,16,16	2.36	3 (23%)	15,22,22	1.74	3 (20%)
2	7QQ	A	1482[B]	-	13,16,16	2.41	3 (23%)	15,22,22	1.90	5 (33%)
2	7QQ	B	1482[A]	-	13,16,16	2.47	4 (30%)	15,22,22	1.94	4 (26%)
2	7QQ	B	1482[B]	-	13,16,16	2.45	4 (30%)	15,22,22	1.91	5 (33%)
2	7QQ	C	1475[A]	-	13,16,16	2.44	4 (30%)	15,22,22	1.90	4 (26%)
2	7QQ	C	1475[B]	-	13,16,16	2.47	4 (30%)	15,22,22	1.89	5 (33%)
2	7QQ	D	1482[A]	-	13,16,16	2.41	3 (23%)	15,22,22	1.81	4 (26%)
2	7QQ	D	1482[B]	-	13,16,16	2.41	4 (30%)	15,22,22	1.89	5 (33%)

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	A	1482[A]	-	-	0/4/6/6	0/2/2/2
2	7QQ	A	1482[B]	-	-	0/4/6/6	0/2/2/2
2	7QQ	B	1482[A]	-	-	0/4/6/6	0/2/2/2
2	7QQ	B	1482[B]	-	-	0/4/6/6	0/2/2/2
2	7QQ	C	1475[A]	-	-	0/4/6/6	0/2/2/2
2	7QQ	C	1475[B]	-	-	0/4/6/6	0/2/2/2
2	7QQ	D	1482[A]	-	-	0/4/6/6	0/2/2/2
2	7QQ	D	1482[B]	-	-	0/4/6/6	0/2/2/2

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1482[A]	7QQ	CAE-CAO	-5.86	1.33	1.40
2	C	1475[A]	7QQ	CAE-CAO	-5.84	1.33	1.40
2	B	1482[B]	7QQ	CAE-CAO	-5.74	1.33	1.40
2	C	1475[B]	7QQ	CAE-CAO	-5.71	1.33	1.40
2	A	1482[A]	7QQ	CAE-CAO	-5.70	1.33	1.40

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1482[A]	7QQ	CAA-OAI-CAL	-4.07	108.59	117.50
2	D	1482[B]	7QQ	CAA-OAI-CAL	-3.70	109.41	117.50
2	C	1475[A]	7QQ	CAA-OAI-CAL	-3.66	109.49	117.50
2	C	1475[A]	7QQ	CAN-CAO-SAJ	-3.51	107.63	112.03
2	C	1475[B]	7QQ	CAN-CAO-SAJ	-3.50	107.63	112.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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, 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	341/368 (92%)	0.04	3 (0%) 84 85	32, 45, 66, 76	0
1	B	322/368 (87%)	0.38	15 (4%) 32 30	36, 60, 82, 94	0
1	C	262/368 (71%)	0.44	15 (5%) 24 22	44, 66, 88, 92	0
1	D	331/368 (89%)	0.23	10 (3%) 51 50	39, 58, 85, 95	0
All	All	1256/1472 (85%)	0.26	43 (3%) 46 44	32, 56, 85, 95	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	ARG	5.7
1	C	354	MET	5.5
1	C	374	VAL	5.4
1	C	391	ALA	3.9
1	B	394	PHE	3.9

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	PTR	B	321	16/17	0.96	0.18	-	58,60,61,61	0
1	PTR	A	321	16/17	0.96	0.19	-	43,44,45,47	0
1	PTR	D	321	16/17	0.96	0.17	-	46,47,48,48	0
1	PTR	C	321	16/17	0.91	0.17	-	63,64,64,65	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	7QQ	A	1482[B]	15/15	0.92	0.31	3.23	65,65,65,66	15
2	7QQ	A	1482[A]	15/15	0.92	0.31	3.16	42,42,43,43	15
2	7QQ	B	1482[B]	15/15	0.94	0.30	2.16	56,57,58,58	15
2	7QQ	B	1482[A]	15/15	0.94	0.30	2.08	46,47,48,48	15
2	7QQ	C	1475[B]	15/15	0.93	0.21	0.52	64,65,66,66	15
2	7QQ	C	1475[A]	15/15	0.93	0.21	0.52	58,59,60,60	15
2	7QQ	D	1482[B]	15/15	0.94	0.19	-0.33	61,62,62,62	15
2	7QQ	D	1482[A]	15/15	0.94	0.19	-0.42	43,43,45,45	15

6.5 Other polymers [i](#)

There are no such residues in this entry.