



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:45 am GMT

PDB ID : 5A3X
Title : DYRK1A in complex with hydroxy benzothiazole fragment
Authors : Rothweiler, U.
Deposited on : 2015-06-03
Resolution : 2.26 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

<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

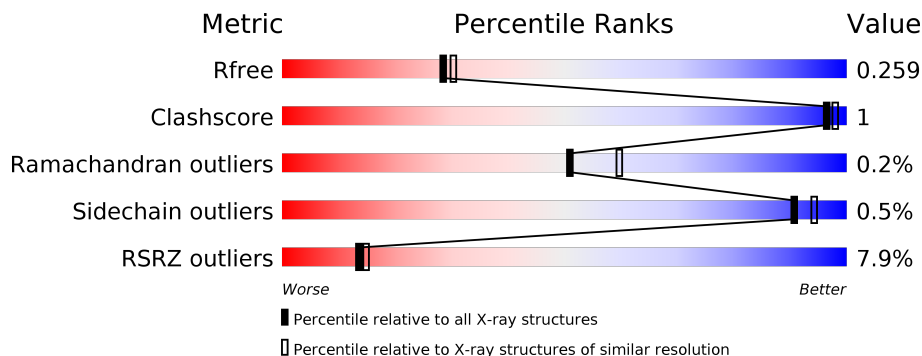
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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 style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="width: 89%; height: 10px; background-color: green; position: relative;"> 89% </div> <div style="width: 7%; height: 10px; background-color: yellow; position: relative;"> 7% </div> </div>
1	B	368	<div> <div style="width: 6%; height: 10px; background-color: red; position: relative;"> 6% </div> <div style="width: 89%; height: 10px; background-color: green; position: relative;"> 89% </div> <div style="width: 7%; height: 10px; background-color: yellow; position: relative;"> 7% </div> </div>
1	C	368	<div> <div style="width: 13%; height: 10px; background-color: red; position: relative;"> 13% </div> <div style="width: 85%; height: 10px; background-color: green; position: relative;"> 85% </div> <div style="width: 5%; height: 10px; background-color: yellow; position: relative;"> 5% </div> <div style="width: 9%; height: 10px; background-color: grey; position: relative;"> 9% </div> </div>
1	D	368	<div> <div style="width: 9%; height: 10px; background-color: red; position: relative;"> 9% </div> <div style="width: 87%; height: 10px; background-color: green; position: relative;"> 87% </div> <div style="width: 10%; height: 10px; background-color: yellow; position: relative;"> 10% </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11323 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.

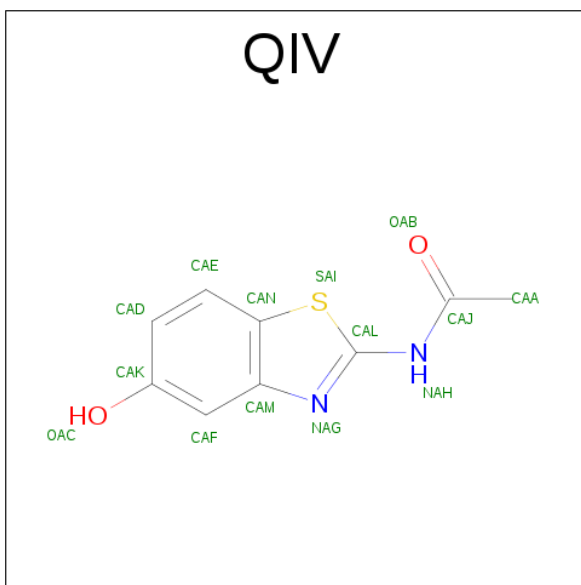
- Molecule 1 is a protein called DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	P	S	0	0	0
			2807	1807	480	502	1	17			
1	B	341	Total	C	N	O	P	S	0	0	0
			2781	1792	474	497	1	17			
1	C	334	Total	C	N	O	P	S	0	0	0
			2730	1757	468	487	1	17			
1	D	332	Total	C	N	O	P	S	0	0	0
			2722	1759	460	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

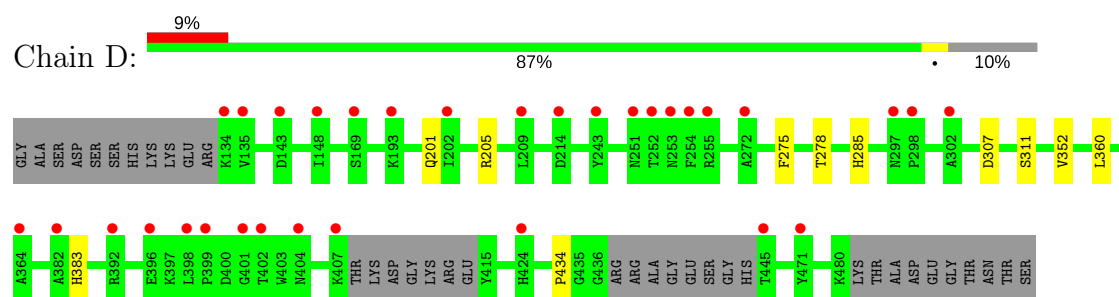
- Molecule 2 is N-(5-OXIDANYL-1,3-BENZOTHAZOL-2-YL)ETHANAMIDE (three-letter code: QIV) (formula: C₉H₈N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			14	9	2	2	1		
2	B	1	Total	C	N	O	S	0	0
			14	9	2	2	1		
2	C	1	Total	C	N	O	S	0	0
			14	9	2	2	1		
2	D	1	Total	C	N	O	S	0	0
			14	9	2	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total	O	0	0
			101	101		
3	B	33	Total	O	0	0
			33	33		
3	C	39	Total	O	0	0
			39	39		
3	D	54	Total	O	0	0
			54	54		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.70Å 88.42Å 229.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 2.26 48.29 – 2.28	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.29-2.26) 99.6 (48.29-2.28)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.235 , 0.259 0.235 , 0.259	Depositor DCC
R_{free} test set	4117 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.216 for k,h,-l	Xtriage
Reported twinning fraction	0.711 for H, K, L 0.289 for K, H, -L	Depositor
Outliers	0 of 82094 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11323	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 2.51% 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: QIV, 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	0.28	0/2855	0.49	0/3848
1	B	0.27	0/2829	0.45	0/3815
1	C	0.27	0/2775	0.47	0/3740
1	D	0.28	0/2768	0.46	0/3732
All	All	0.28	0/11227	0.47	0/15135

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	2807	0	2809	9	0
1	B	2781	0	2776	9	0
1	C	2730	0	2724	9	0
1	D	2722	0	2727	6	0
2	A	14	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	0	0
2	D	14	0	0	1	0
3	A	101	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	0	0	0
3	C	39	0	0	0	0
3	D	54	0	0	0	0
All	All	11323	0	11036	27	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 1.

All (27) 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:374:VAL:HG11	1:A:405:LEU:HD11	1.82	0.61
1:B:314:LEU:HD22	1:B:338:TYR:CE2	2.46	0.51
1:D:352:VAL:HG11	1:D:360:LEU:HD13	1.93	0.51
1:A:201:GLN:HE22	1:B:318:ILE:HG23	1.78	0.49
1:A:472:TYR:OH	1:D:383:HIS:HB2	2.12	0.49
1:C:287:ASP:OD1	1:C:324:SER:OG	2.24	0.48
1:B:249:LEU:HD22	1:B:357:GLY:HA2	1.97	0.47
1:C:388:ALA:HB3	1:C:391:ALA:HB2	1.97	0.47
1:D:275:PHE:O	1:D:278:THR:HG23	2.15	0.46
1:A:201:GLN:HE22	1:B:318:ILE:CG2	2.28	0.46
1:C:164:LEU:HD21	1:C:167:LYS:HD2	1.97	0.46
1:A:169:SER:OG	1:B:193:LYS:NZ	2.49	0.45
1:B:282:SER:HB2	1:C:315:GLY:O	2.17	0.45
1:C:352:VAL:HG11	1:C:360:LEU:HD13	1.99	0.44
1:A:161:ILE:HG23	1:A:174:VAL:HG21	1.99	0.44
1:D:285:HIS:NE2	1:D:307:ASP:O	2.51	0.44
1:C:314:LEU:HD21	1:C:338:TYR:CE2	2.53	0.43
1:A:394:PHE:HB2	1:A:395:PHE:CD2	2.53	0.43
1:C:194:LYS:NZ	1:D:311:SER:O	2.52	0.42
1:C:244:ASN:HA	1:C:294:LEU:HA	2.01	0.42
2:D:1481:QIV:SAI	2:D:1481:QIV:OAB	2.78	0.41
1:C:158:ARG:O	1:C:179:ARG:HG2	2.21	0.41
1:A:147:TYR:OH	1:A:231:ARG:NH1	2.54	0.41
1:B:331:GLU:HB2	1:B:336:MET:HB2	2.03	0.41
1:B:398:LEU:HB3	1:B:399:PRO:CD	2.51	0.41
1:D:201:GLN:O	1:D:205:ARG:HG3	2.22	0.40
1:A:311:SER:O	1:B:194:LYS:NZ	2.46	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	338/368 (92%)	322 (95%)	15 (4%)	1 (0%)	44	50
1	B	336/368 (91%)	315 (94%)	21 (6%)	0	100	100
1	C	327/368 (89%)	309 (94%)	18 (6%)	0	100	100
1	D	325/368 (88%)	312 (96%)	12 (4%)	1 (0%)	44	50
All	All	1326/1472 (90%)	1258 (95%)	66 (5%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	GLN
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	303/324 (94%)	302 (100%)	1 (0%)	94	97
1	B	299/324 (92%)	298 (100%)	1 (0%)	94	97
1	C	294/324 (91%)	290 (99%)	4 (1%)	71	81
1	D	295/324 (91%)	295 (100%)	0	100	100
All	All	1191/1296 (92%)	1185 (100%)	6 (0%)	91	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	CYS
1	B	394	PHE
1	C	226	ARG
1	C	286	CYS
1	C	402	THR
1	C	417	PRO

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

Mol	Chain	Res	Type
1	A	201	GLN
1	A	387	GLN
1	D	387	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	0.70	0	19,22,24	0.77	0
1	PTR	B	321	1	15,16,17	0.66	0	19,22,24	0.77	0
1	PTR	C	321	1	15,16,17	0.66	0	19,22,24	0.82	0
1	PTR	D	321	1	15,16,17	0.61	0	19,22,24	0.78	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](#)

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	QIV	A	1482	-	12,15,15	2.47	2 (16%)	14,21,21	1.60	5 (35%)
2	QIV	B	1482	-	12,15,15	2.37	2 (16%)	14,21,21	1.71	5 (35%)
2	QIV	C	1482	-	12,15,15	2.41	2 (16%)	14,21,21	1.65	5 (35%)
2	QIV	D	1481	-	12,15,15	2.33	2 (16%)	14,21,21	1.78	5 (35%)

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	QIV	A	1482	-	-	0/2/4/4	0/2/2/2
2	QIV	B	1482	-	-	0/2/4/4	0/2/2/2
2	QIV	C	1482	-	-	0/2/4/4	0/2/2/2
2	QIV	D	1481	-	-	0/2/4/4	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1482	QIV	CAE-CAN	-6.11	1.33	1.40
2	C	1482	QIV	CAE-CAN	-5.68	1.33	1.40
2	B	1482	QIV	CAE-CAN	-5.55	1.33	1.40
2	D	1481	QIV	CAE-CAN	-5.43	1.34	1.40
2	C	1482	QIV	CAF-CAM	-5.06	1.34	1.41
2	B	1482	QIV	CAF-CAM	-4.96	1.34	1.41
2	A	1482	QIV	CAF-CAM	-4.90	1.34	1.41
2	D	1481	QIV	CAF-CAM	-4.88	1.34	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1482	QIV	CAM-CAN-SAI	-3.10	108.14	112.03
2	D	1481	QIV	CAM-CAN-SAI	-2.93	108.35	112.03
2	C	1482	QIV	CAM-CAN-SAI	-2.87	108.42	112.03
2	A	1482	QIV	CAM-CAN-SAI	-2.50	108.89	112.03
2	B	1482	QIV	CAD-CAE-CAN	2.05	120.38	118.81
2	B	1482	QIV	CAN-CAM-NAG	2.12	112.92	108.04
2	A	1482	QIV	CAN-CAM-NAG	2.14	112.97	108.04
2	C	1482	QIV	CAN-CAM-NAG	2.15	113.00	108.04
2	C	1482	QIV	CAD-CAE-CAN	2.15	120.45	118.81
2	D	1481	QIV	CAN-CAM-NAG	2.18	113.07	108.04
2	A	1482	QIV	OAB-CAJ-NAH	2.25	125.98	123.06
2	C	1482	QIV	OAB-CAJ-NAH	2.30	126.06	123.06
2	D	1481	QIV	OAB-CAJ-NAH	2.31	126.06	123.06
2	D	1481	QIV	CAD-CAE-CAN	2.34	120.59	118.81
2	A	1482	QIV	CAD-CAE-CAN	2.42	120.66	118.81
2	B	1482	QIV	OAB-CAJ-NAH	2.49	126.30	123.06
2	A	1482	QIV	CAK-CAF-CAM	2.51	120.83	119.17
2	C	1482	QIV	CAK-CAF-CAM	2.68	120.94	119.17
2	B	1482	QIV	CAK-CAF-CAM	2.76	120.99	119.17
2	D	1481	QIV	CAK-CAF-CAM	3.23	121.31	119.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1481	QIV	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, 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	342/368 (92%)	0.20	4 (1%) 79 81	22, 35, 52, 66	0
1	B	340/368 (92%)	0.73	23 (6%) 18 20	32, 54, 76, 95	0
1	C	333/368 (90%)	0.86	47 (14%) 3 3	31, 51, 81, 84	0
1	D	331/368 (89%)	0.71	32 (9%) 8 9	30, 45, 68, 79	0
All	All	1346/1472 (91%)	0.62	106 (7%) 13 15	22, 47, 75, 95	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	445	THR	6.2
1	C	402	THR	5.4
1	C	377	LEU	4.8
1	C	481	LYS	4.8
1	B	406	LYS	4.5
1	C	404	ASN	4.5
1	B	401	GLY	4.3
1	A	481	LYS	4.1
1	D	297	ASN	3.9
1	C	386	ASP	3.9
1	C	379	ILE	3.8
1	B	315	GLY	3.8
1	C	376	VAL	3.8
1	D	401	GLY	3.7
1	C	382	ALA	3.5
1	D	135	VAL	3.5
1	D	399	PRO	3.5
1	B	263	ARG	3.5
1	C	449	TYR	3.4
1	D	251	ASN	3.4
1	C	419	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	388	ALA	3.3
1	A	136	TYR	3.2
1	C	427	LEU	3.2
1	B	480	LYS	3.2
1	C	385	LEU	3.2
1	C	440	GLY	3.2
1	C	435	GLY	3.2
1	D	143	ASP	3.2
1	A	243	TYR	3.1
1	B	182	GLN	3.1
1	D	148	ILE	3.1
1	C	299	LYS	3.0
1	D	243	TYR	3.0
1	C	145	TYR	3.0
1	C	220	TYR	3.0
1	C	472	TYR	3.0
1	B	212	LYS	3.0
1	C	424	HIS	3.0
1	C	436	GLY	2.9
1	B	421	ARG	2.9
1	C	315	GLY	2.9
1	C	381	PRO	2.9
1	C	334	LEU	2.8
1	D	407	LYS	2.8
1	D	402	THR	2.8
1	C	135	VAL	2.7
1	D	398	LEU	2.7
1	D	298	PRO	2.7
1	B	326	PHE	2.7
1	D	253	ASN	2.7
1	B	427	LEU	2.6
1	D	404	ASN	2.6
1	B	398	LEU	2.6
1	D	392	ARG	2.6
1	C	420	THR	2.5
1	C	480	LYS	2.5
1	C	384	ILE	2.5
1	C	396	GLU	2.5
1	A	480	LYS	2.5
1	B	314	LEU	2.5
1	C	397	LYS	2.5
1	C	475	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	272	ALA	2.4
1	D	471	TYR	2.4
1	C	392	ARG	2.4
1	B	452	PHE	2.4
1	C	373	ILE	2.4
1	C	442	SER	2.4
1	C	336	MET	2.4
1	C	478	PHE	2.4
1	C	426	ILE	2.4
1	D	396	GLU	2.3
1	D	193	LYS	2.3
1	C	422	LYS	2.3
1	C	318	ILE	2.3
1	D	214	ASP	2.3
1	C	474	LEU	2.3
1	D	252	THR	2.3
1	B	393	LYS	2.3
1	B	400	ASP	2.2
1	B	308	PHE	2.2
1	D	254	PHE	2.2
1	B	396	GLU	2.2
1	D	169	SER	2.2
1	C	313	GLN	2.2
1	D	202	ILE	2.2
1	B	136	TYR	2.2
1	B	460	LEU	2.2
1	D	255	ARG	2.2
1	C	417	PRO	2.2
1	C	466	THR	2.2
1	C	394	PHE	2.1
1	D	302	ALA	2.1
1	B	313	GLN	2.1
1	B	243	TYR	2.1
1	D	134	LYS	2.1
1	C	316	GLN	2.1
1	B	207	LEU	2.0
1	D	382	ALA	2.0
1	B	330	PRO	2.0
1	C	477	SER	2.0
1	D	424	HIS	2.0
1	C	360	LEU	2.0
1	D	209	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	364	ALA	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. 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	0.94	0.17	-	46,48,49,49	0
1	PTR	A	321	16/17	0.96	0.13	-	28,29,30,30	0
1	PTR	D	321	16/17	0.94	0.12	-	32,36,37,38	0
1	PTR	C	321	16/17	0.94	0.15	-	48,50,51,51	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	QIV	B	1482	14/14	0.89	0.15	-0.63	46,47,49,50	0
2	QIV	D	1481	14/14	0.94	0.12	-1.47	39,40,42,42	0
2	QIV	A	1482	14/14	0.94	0.12	-1.56	31,32,34,34	0
2	QIV	C	1482	14/14	0.96	0.12	-1.97	41,41,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.