WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 10:49 pm BST

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

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

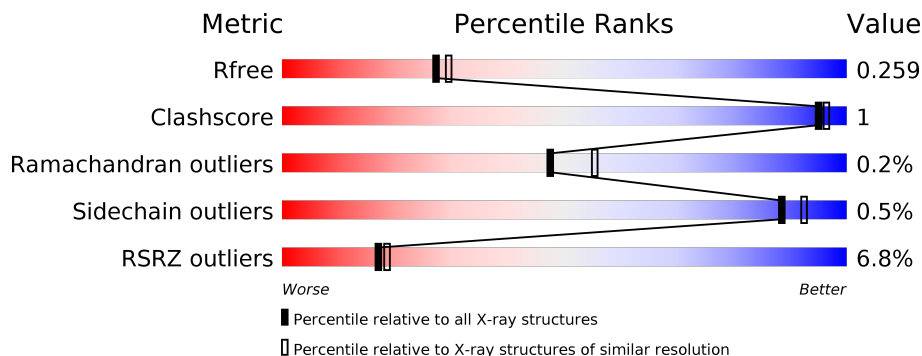|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.26 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	Percentile Ranks	Value
Rfree		0.259
Clashscore		1
Ramachandran outliers		0.2%
Sidechain outliers		0.5%
RSRZ outliers		6.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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 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 <=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	2% 89% • 7%
1	B	368	7% 89% • 7%
1	C	368	11% 85% 5% 9%
1	D	368	4% 87% • 10%

2 Entry composition (i)

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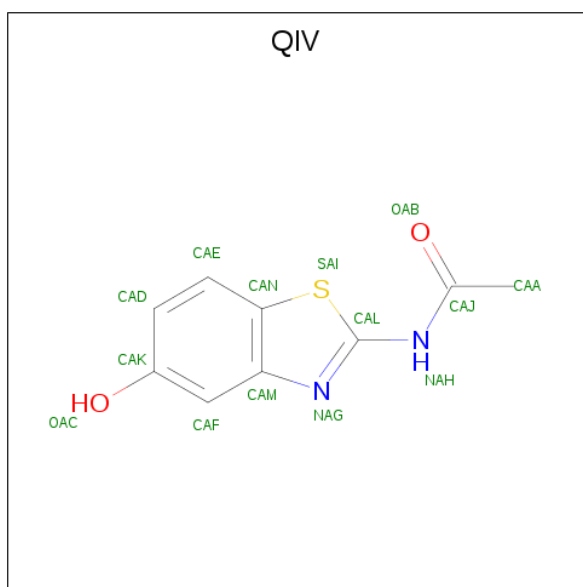
- Molecule 1 is a protein called DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A.

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-benzothiazol-2-yl)ethanamide (three-letter code: QIV) (formula: $C_9H_8N_2O_2S$).

QIV

OAB

CAE

CAD

SAI

CAN

S

O

CAA

CAL

CAJ

CAK

N

H

HO

CAM

N

NAH

OAC

CAF

NAG

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			
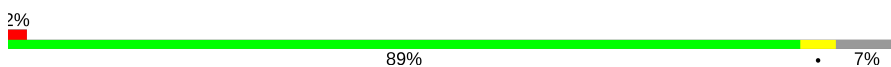
- Molecule 3 is water.

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		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.
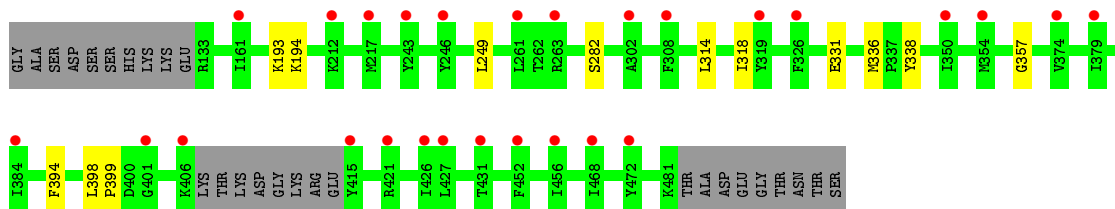
- Molecule 1: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A
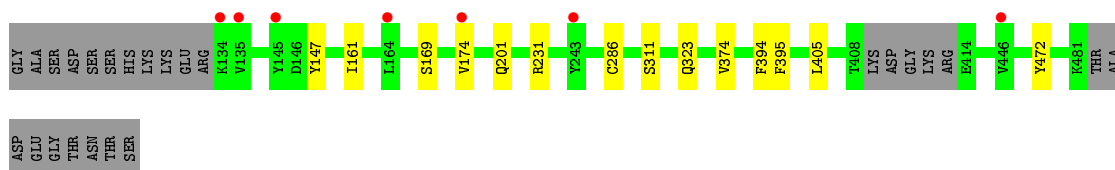
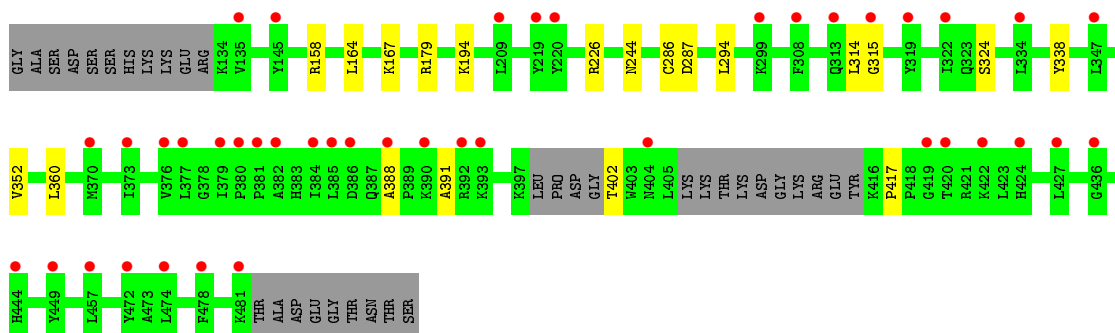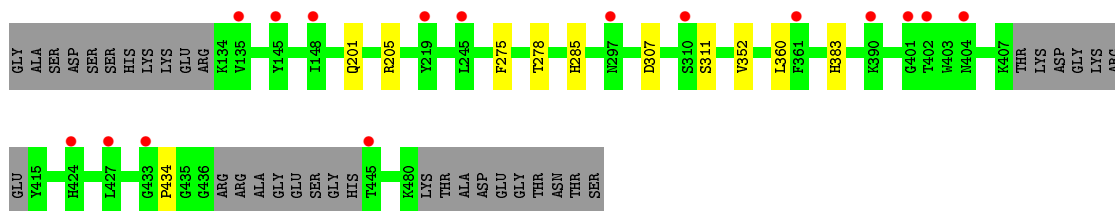- Molecule 1: DUAL SPECIFICITY TYROSINE-PHOSPHORYLATION-REGULATED KINASE 1A

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

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

Chain D:

4 Data and refinement statistics (i)

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) 97.7 (48.29-2.28)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 20.3	EDS
L-test for twinning [2]	$< |L| > = 0.40, < L^2 > = 0.23$	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	0.92	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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

Continued from previous page...

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.

The worst 5 of 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

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%)	41	46
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%)	41	46
All	All	1326/1472 (90%)	1258 (95%)	66 (5%)	2 (0%)	47	55

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%)	92	95
1	B	299/324 (92%)	298 (100%)	1 (0%)	92	95
1	C	294/324 (91%)	290 (99%)	4 (1%)	67	76
1	D	295/324 (91%)	295 (100%)	0	100	100
All	All	1191/1296 (92%)	1185 (100%)	6 (0%)	88	92

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

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

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 (i)

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	B	321	1	15,16,17	0.80	0	19,22,24	0.69	0
1	PTR	A	321	1	15,16,17	0.79	0	19,22,24	0.73	0
1	PTR	D	321	1	15,16,17	0.74	0	19,22,24	0.71	0
1	PTR	C	321	1	15,16,17	0.79	0	19,22,24	0.71	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	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
1	PTR	C	321	1	-	1/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	321	PTR	O-C-CA-CB
1	C	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 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	B	1482	-	12,15,15	1.83	2 (16%)	12,21,21	1.57	3 (25%)
2	QIV	D	1481	-	12,15,15	1.80	3 (25%)	12,21,21	1.58	3 (25%)
2	QIV	A	1482	-	12,15,15	1.84	2 (16%)	12,21,21	1.43	3 (25%)
2	QIV	C	1482	-	12,15,15	1.85	2 (16%)	12,21,21	1.50	3 (25%)

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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1482	QIV	CAF-CAM	-4.89	1.34	1.41
2	B	1482	QIV	CAF-CAM	-4.79	1.34	1.41
2	A	1482	QIV	CAF-CAM	-4.73	1.34	1.41
2	D	1481	QIV	CAF-CAM	-4.71	1.34	1.41
2	A	1482	QIV	CAE-CAN	-2.39	1.33	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1482	QIV	CAM-CAN-SAI	-2.80	108.14	111.85
2	D	1481	QIV	CAM-CAN-SAI	-2.64	108.35	111.85
2	C	1482	QIV	CAM-CAN-SAI	-2.58	108.42	111.85
2	B	1482	QIV	OAB-CAJ-NAH	2.48	126.30	123.04
2	D	1481	QIV	OAB-CAJ-NAH	2.30	126.06	123.04

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 (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(Å²)	Q<0.9
1	A	342/368 (92%)	0.24	7 (2%)	65	68	22, 35, 52, 66	0
1	B	340/368 (92%)	0.69	27 (7%)	12	14	32, 54, 76, 95	0
1	C	333/368 (90%)	0.79	42 (12%)	3	3	31, 51, 81, 84	0
1	D	331/368 (89%)	0.61	16 (4%)	30	33	30, 45, 68, 79	0
All	All	1346/1472 (91%)	0.58	92 (6%)	17	18	22, 47, 75, 95	0

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	381	PRO	4.7
1	B	401	GLY	4.7
1	C	376	VAL	4.2
1	C	427	LEU	3.7
1	B	379	ILE	3.7

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, 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(Å²)	Q<0.9
1	PTR	B	321	16/17	0.92	0.18	46,48,49,49	0
1	PTR	D	321	16/17	0.93	0.11	32,36,37,38	0
1	PTR	C	321	16/17	0.93	0.16	48,50,51,51	0
1	PTR	A	321	16/17	0.97	0.13	28,29,30,30	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, 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(Å^2)	Q<0.9
2	QIV	B	1482	14/14	0.88	0.18	46,47,49,50	0
2	QIV	D	1481	14/14	0.93	0.14	39,40,42,42	0
2	QIV	A	1482	14/14	0.94	0.15	31,32,34,34	0
2	QIV	C	1482	14/14	0.94	0.14	41,41,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.