Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:13 PM EDT

PDB ID	:	1Q8T
Title	:	The Catalytic Subunit of cAMP-dependent Protein Kinase (PKA) in Complex with Rho-kinase Inhibitor Y-27632
Authors	:	Breitenlechner, C.; Gassel, M.; Hidaka, H.; Kinzel, V.; Huber, R.; Engh, R.A.; Bossemeyer, D.
Deposited on	:	2003-08-22
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

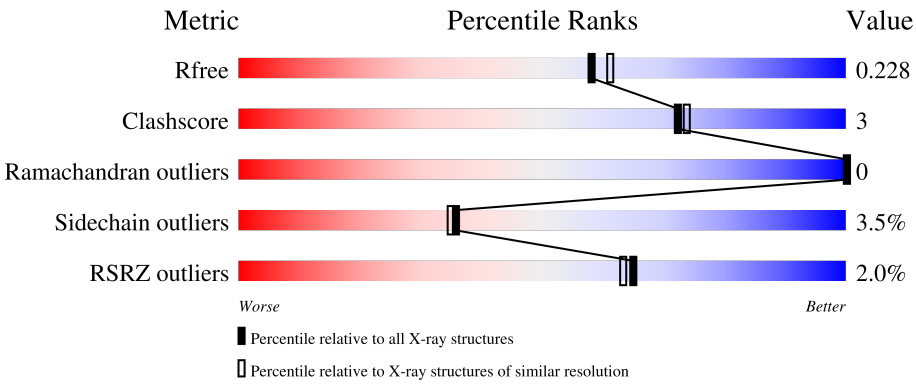
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

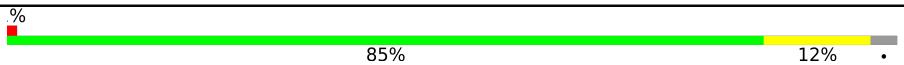
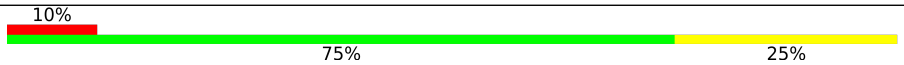
The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 >=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	350	
2	B	20	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3244 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 cAMP-dependent protein kinase, alpha-catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	341	2849	1838	477	522	3	9	35	7	0

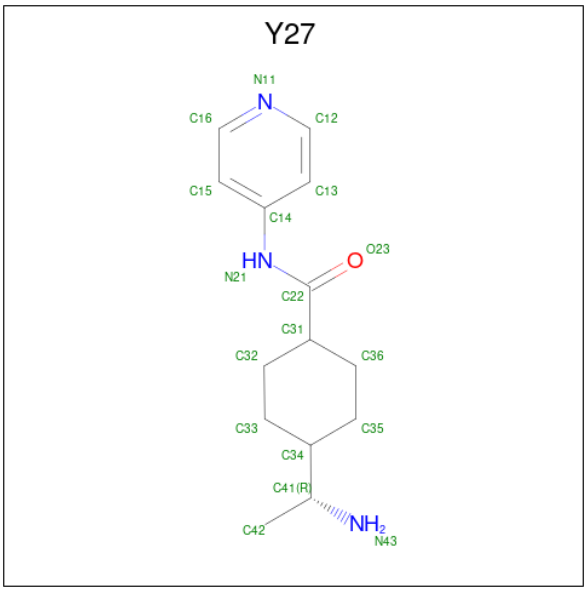
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	SEP	SER	MODIFIED RESIDUE	UNP P00517
A	197	TPO	THR	MODIFIED RESIDUE	UNP P00517
A	338	SEP	SER	MODIFIED RESIDUE	UNP P00517

- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor, alpha form.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	20	157	94	32	31	0	0	0

- Molecule 3 is (R)-TRANS-4-(1-AMINOETHYL)-N-(4-PYRIDYL) CYCLOHEXANECARB OXAMIDE (three-letter code: Y27) (formula: $C_{14}H_{21}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	18	14	3	1	0	0

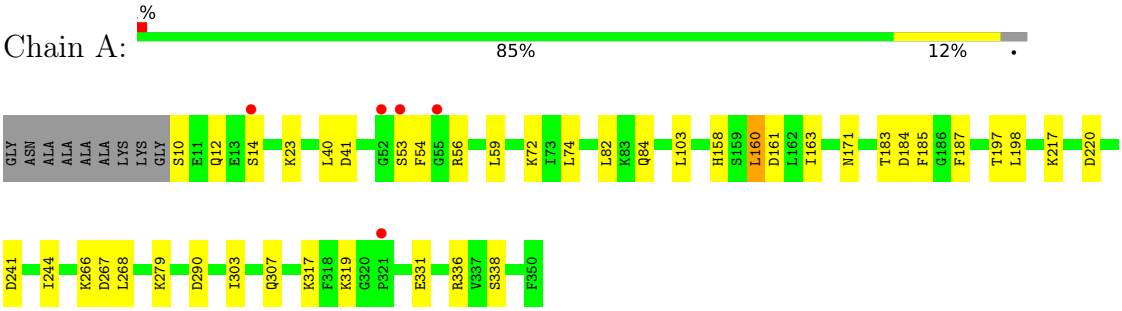
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	196	196	196	0	0
			Total	O		
4	B	24	24	24	0	0

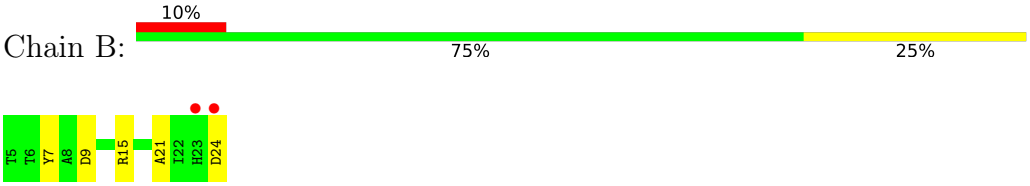
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: cAMP-dependent protein kinase, alpha-catalytic subunit



• Molecule 2: cAMP-dependent protein kinase inhibitor, alpha form



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.03Å 76.61Å 80.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.83 – 2.00 15.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (15.83-2.00) 97.7 (15.83-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.176 , 0.229 0.178 , 0.228	Depositor DCC
R_{free} test set	3104 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3244	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: SEP, TPO, Y27

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	0.77	4/2923 (0.1%)	0.85	9/3938 (0.2%)
2	B	0.64	0/159	0.99	2/212 (0.9%)
All	All	0.76	4/3082 (0.1%)	0.85	11/4150 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	GLN	CB-CG	-10.89	1.23	1.52
1	A	336	ARG	CB-CG	9.68	1.78	1.52
1	A	317	LYS	CG-CD	-7.38	1.27	1.52
1	A	279	LYS	CG-CD	6.67	1.75	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	12	GLN	CA-CB-CG	12.71	141.37	113.40
1	A	336	ARG	CA-CB-CG	-8.18	95.41	113.40
1	A	41	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	317	LYS	CB-CG-CD	6.58	128.71	111.60
1	A	161	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	12	GLN	CB-CG-CD	-6.31	95.20	111.60
1	A	241	ASP	CB-CG-OD2	5.85	123.56	118.30
2	B	9	ASP	CB-CG-OD2	5.85	123.56	118.30
2	B	24	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	290	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	267	ASP	CB-CG-OD2	5.42	123.17	118.30

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	2849	0	2815	19	0
2	B	157	0	146	2	0
3	A	18	0	21	3	0
4	A	196	0	0	1	0
4	B	24	0	0	1	0
All	All	3244	0	2982	20	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 3.

All (20) 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:72:LYS:HE2	1:A:74:LEU:HD21	1.82	0.62
1:A:171:ASN:OD1	3:A:930:Y27:H423	2.02	0.58
1:A:163:ILE:HG22	1:A:217:LYS:CG	2.34	0.57
1:A:163:ILE:HG22	1:A:217:LYS:HG2	1.91	0.52
1:A:187:PHE:HE2	2:B:21:ALA:HB1	1.74	0.52
1:A:158:HIS:HE1	1:A:220:ASP:OD2	1.92	0.52
1:A:103:LEU:HD22	1:A:185:PHE:HZ	1.74	0.52
1:A:56[A]:ARG:NH2	1:A:331:GLU:O	2.46	0.49
1:A:163:ILE:HG22	1:A:217:LYS:HG3	1.94	0.48
1:A:183[B]:THR:CG2	3:A:930:Y27:H362	2.44	0.47
1:A:103:LEU:HD22	1:A:185:PHE:CZ	2.52	0.45
1:A:54:PHE:HB2	1:A:74:LEU:HD22	1.99	0.44
1:A:184:ASP:OD1	3:A:930:Y27:H422	2.19	0.43
1:A:54:PHE:CZ	1:A:84:GLN:HG3	2.53	0.43
2:B:7:TYR:OH	4:B:41:HOH:O	2.21	0.42
1:A:158:HIS:HD2	4:A:998:HOH:O	2.03	0.42
1:A:23:LYS:HE3	1:A:160:LEU:HA	2.01	0.41
1:A:163:ILE:HD13	1:A:163:ILE:HG21	1.67	0.41
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.95	0.40
1:A:303:ILE:O	1:A:307:GLN:HG3	2.22	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	344/350 (98%)	336 (98%)	8 (2%)	0	100	100
2	B	18/20 (90%)	18 (100%)	0	0	100	100
All	All	362/370 (98%)	354 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	306/302 (101%)	296 (97%)	10 (3%)	38	37
2	B	15/15 (100%)	14 (93%)	1 (7%)	16	11
All	All	321/317 (101%)	310 (97%)	11 (3%)	36	36

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

Mol	Chain	Res	Type
1	A	14	SER
1	A	40	LEU
1	A	53	SER
1	A	59	LEU
1	A	160	LEU
1	A	198	LEU
1	A	244	ILE
1	A	266	LYS

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Mol	Chain	Res	Type
1	A	268	LEU
1	A	319	LYS
2	B	15	ARG

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

Mol	Chain	Res	Type
1	A	62	HIS
1	A	113	ASN
1	A	158	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)

3 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	SEP	A	338	1	8,9,10	1.60	1 (12%)	8,12,14	2.31	2 (25%)
1	SEP	A	10	1	8,9,10	1.74	2 (25%)	8,12,14	1.43	1 (12%)
1	TPO	A	197	1	8,10,11	1.25	1 (12%)	10,14,16	0.99	1 (10%)

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	SEP	A	338	1	-	3/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	10	1	-	0/5/8/10	-
1	TPO	A	197	1	-	1/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	SEP	P-O1P	3.67	1.62	1.50
1	A	338	SEP	P-O1P	3.31	1.61	1.50
1	A	197	TPO	P-O1P	2.43	1.58	1.50
1	A	10	SEP	P-O2P	2.08	1.62	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	338	SEP	OG-CB-CA	5.49	113.49	108.14
1	A	10	SEP	OG-CB-CA	3.33	111.38	108.14
1	A	338	SEP	OG-P-O1P	2.60	113.77	106.47
1	A	197	TPO	P-OG1-CB	-2.32	116.20	123.21

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	197	TPO	O-C-CA-CB
1	A	338	SEP	CB-OG-P-O2P
1	A	338	SEP	CA-CB-OG-P
1	A	338	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
3	Y27	A	930	-	19,19,19	1.28	3 (15%)	23,25,25	1.21	4 (17%)

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
3	Y27	A	930	-	-	2/12/22/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	930	Y27	C22-N21	3.15	1.42	1.35
3	A	930	Y27	C13-C14	2.20	1.42	1.39
3	A	930	Y27	C41-N43	2.02	1.51	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	930	Y27	C36-C35-C34	-2.38	106.88	112.24
3	A	930	Y27	C12-N11-C16	2.33	122.34	116.85
3	A	930	Y27	C13-C12-N11	-2.22	119.76	123.62
3	A	930	Y27	C16-C15-C14	-2.08	116.09	118.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	930	Y27	C33-C34-C41-N43
3	A	930	Y27	C33-C34-C41-C42

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	930	Y27	3	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(Å^2)	Q<0.9
1	A	338/350 (96%)	-0.08	5 (1%)	73	72	22, 36, 54, 68	28 (8%)
2	B	20/20 (100%)	-0.16	2 (10%)	7	6	26, 30, 46, 49	2 (10%)
All	All	358/370 (96%)	-0.08	7 (1%)	65	63	22, 36, 54, 68	30 (8%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	321	PRO	3.4
2	B	24	ASP	3.0
1	A	14	SER	2.8
2	B	23	HIS	2.7
1	A	52	GLY	2.5
1	A	55	GLY	2.4
1	A	53	SER	2.1

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(Å^2)	Q<0.9
1	SEP	A	10	10/11	0.71	0.31	68,70,78,78	0
1	SEP	A	338	10/11	0.92	0.11	54,54,59,60	0
1	TPO	A	197	11/12	0.99	0.07	26,27,29,31	0

6.3 Carbohydrates (i)

There are no monosaccharides 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
3	Y27	A	930	18/18	0.93	0.14	27,38,43,44	0

6.5 Other polymers (i)

There are no such residues in this entry.