W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 09:15 AM GMT

PDB ID : 3DDQ

Title : Structure of phosphorylated Thr160 CDK2/cyclin A in complex with the inhibitor roscovitine

Authors : Echalier, A.; Endicott, J.A.

Deposited on : 2008-06-06

Resolution : 1.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
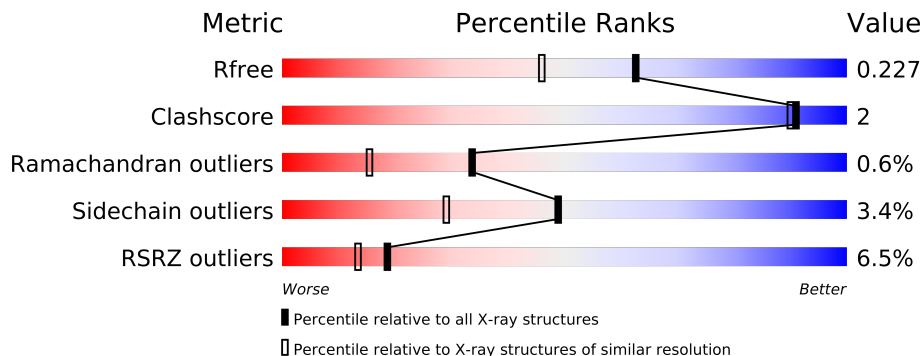A user guide is available at http://wwpdb.org/ValidationPDFNotes.html

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 1.80 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		0.227
Clashscore		2
Ramachandran outliers		0.6%
Sidechain outliers		3.4%
RSRZ outliers		6.5%

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}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	299	
1	C	299	
2	B	269	
2	D	269	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SGM	B	1	-	X
4	SGM	B	440	-	X
4	SGM	D	1	-	X

WORLDWIDE
wwPDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 9800 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Cell division protein kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total 2405	C 1562	N 410	O 424	P 1	S 8	0	2	0
1	C	267	Total 2179	C 1411	N 377	O 383	P 1	S 7	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP P24941
C	0	SER	-	EXPRESSION TAG	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total 2135	C 1385	N 347	O 393	S 10	0	4	0
2	D	269	Total 2188	C 1414	N 366	O 398	S 10	0	1	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	433	HIS	-	EXPRESSION TAG	UNP P30274
B	434	HIS	-	EXPRESSION TAG	UNP P30274
B	435	HIS	-	EXPRESSION TAG	UNP P30274
B	436	HIS	-	EXPRESSION TAG	UNP P30274
B	437	HIS	-	EXPRESSION TAG	UNP P30274
B	438	HIS	-	EXPRESSION TAG	UNP P30274
B	439	HIS	-	EXPRESSION TAG	UNP P30274
D	433	HIS	-	EXPRESSION TAG	UNP P30274
D	434	HIS	-	EXPRESSION TAG	UNP P30274
D	435	HIS	-	EXPRESSION TAG	UNP P30274

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Chain	Residue	Modelled	Actual	Comment	Reference
D	436	HIS	-	EXPRESSION TAG	UNP P30274
D	437	HIS	-	EXPRESSION TAG	UNP P30274
D	438	HIS	-	EXPRESSION TAG	UNP P30274
D	439	HIS	-	EXPRESSION TAG	UNP P30274

- Molecule 3 is R-ROSCOVITINE (three-letter code: RRC) (formula: $C_{19}H_{26}N_6O$).
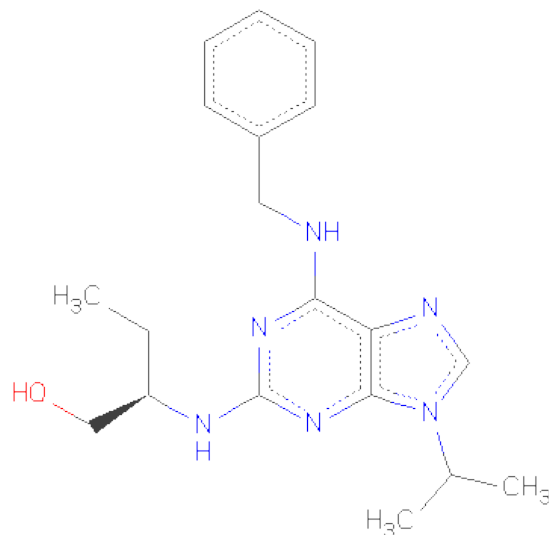
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 26	C 19	N 6	O 1	0	0
3	C	1	Total 26	C 19	N 6	O 1	0	0

- Molecule 4 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: $C_3H_8O_2S$).
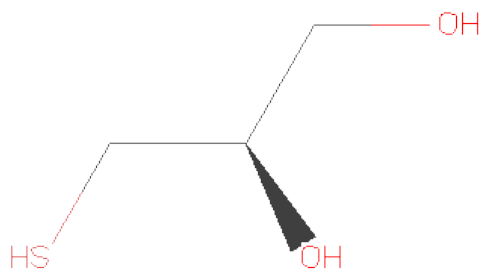
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 6	C 3	O 2	S 1	0	0
4	B	1	Total 6	C 3	O 2	S 1	0	0
4	D	1	Total 6	C 3	O 2	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	265	Total 265	O 265	0	0
5	B	219	Total 219	O 219	0	0
5	C	153	Total 153	O 153	0	0
5	D	186	Total 186	O 186	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
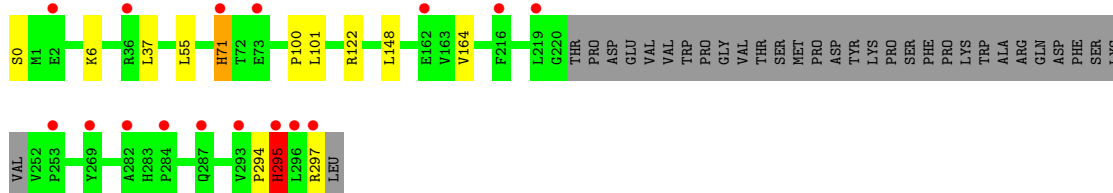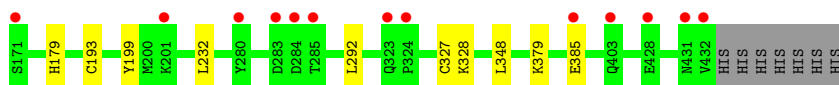
- Molecule 1: Cell division protein kinase 2

Chain A:
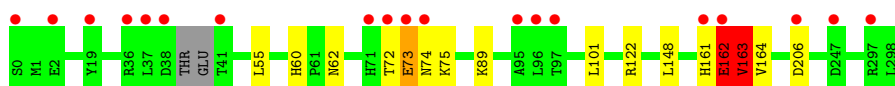
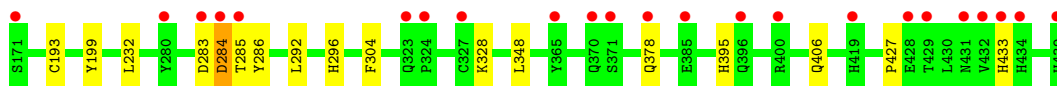- Molecule 1: Cell division protein kinase 2

Chain C:

- Molecule 2: Cyclin-A2

Chain B:

- Molecule 2: Cyclin-A2

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	74.42Å 133.38Å 147.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 19.90 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.0 (20.00-1.80) 90.0 (19.90-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.87 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.229 0.194 , 0.227	Depositor DCC
R_{free} test set	4947 reflections (4.21%)	DCC
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 37.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	0 of 122533 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9800	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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: TPO, RRC, SGM

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	0.50	0/2460	0.62	4/3334 (0.1%)
1	C	0.40	0/2232	0.58	0/3019
2	B	0.40	0/2198	0.53	0/2989
2	D	0.38	0/2248	0.53	0/3056
All	All	0.42	0/9138	0.57	4/12398 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162[A]	GLU	CA-C-N	-5.35	105.42	117.20
1	A	162[B]	GLU	CA-C-N	-5.35	105.42	117.20
1	A	162[A]	GLU	CA-C-O	5.21	131.03	120.10
1	A	162[B]	GLU	CA-C-O	5.21	131.03	120.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162[A]	GLU	Mainchain
1	A	162[B]	GLU	Mainchain
1	C	294	PRO	Peptide
1	C	37	LEU	Peptide

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2405	0	0	5	0
1	C	2179	0	0	4	0
2	B	2135	0	0	3	0
2	D	2188	0	0	8	0
3	A	26	0	0	0	0
3	C	26	0	0	0	0
4	B	12	0	0	2	0
4	D	6	0	0	1	0
5	A	265	0	0	1	0
5	B	219	0	0	0	0
5	C	153	0	0	1	0
5	D	186	0	0	4	0
All	All	9800	0	0	18	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (18) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:193:CYS:SG	4:D:1:SGM:S1	2.36	1.23
2:B:193:CYS:SG	4:B:1:SGM:S1	2.51	1.09
2:B:327:CYS:SG	4:B:440:SGM:S1	2.68	0.92
1:C:71[A]:HIS:CD2	2:D:296:HIS:CE1	2.90	0.59
1:A:73:GLU:CG	1:A:74:ASN:N	2.68	0.56
2:D:406:GLN:NE2	5:D:569:HOH:O	2.43	0.51
1:A:161:HIS:CD2	5:A:411:HOH:O	2.65	0.49
1:C:0:SER:N	5:C:418:HOH:O	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:179[B]:HIS:CE1	2:B:379:LYS:NZ	2.84	0.45
1:C:100:PRO:CD	1:C:295:HIS:CD2	3.00	0.45
2:D:286:TYR:N	5:D:536:HOH:O	2.49	0.45
2:D:284:ASP:N	5:D:531:HOH:O	2.49	0.45
2:D:285:THR:N	5:D:536:HOH:O	2.50	0.44
1:A:162[B]:GLU:CG	1:A:163:VAL:N	2.80	0.44
2:D:395:HIS:CE1	2:D:427:PRO:O	2.73	0.42
1:C:71[A]:HIS:CE1	2:D:304:PHE:CE2	3.08	0.42
1:A:60:HIS:CD2	1:A:62:ASN:N	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	294/299 (98%)	284 (97%)	5 (2%)	5 (2%)	14	2
1	C	267/299 (89%)	256 (96%)	9 (3%)	2 (1%)	30	13
2	B	264/269 (98%)	263 (100%)	1 (0%)	0	100	100
2	D	268/269 (100%)	266 (99%)	2 (1%)	0	100	100
All	All	1093/1136 (96%)	1069 (98%)	17 (2%)	7 (1%)	33	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	A	162[A]	GLU
1	A	162[B]	GLU
1	A	163	VAL
1	A	164	VAL
1	C	164	VAL
1	C	295	HIS

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	263/263 (100%)	252 (96%)	11 (4%)	40	20
1	C	238/263 (90%)	229 (96%)	9 (4%)	44	24
2	B	239/242 (99%)	233 (98%)	6 (2%)	60	42
2	D	243/242 (100%)	234 (96%)	9 (4%)	45	26
All	All	983/1010 (97%)	948 (96%)	35 (4%)	49	27

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	72	THR
1	A	75	LYS
1	A	89	LYS
1	A	101	LEU
1	A	122	ARG
1	A	148	LEU
1	A	162[A]	GLU
1	A	162[B]	GLU
1	A	163	VAL
1	A	206	ASP
2	B	199	TYR
2	B	232	LEU
2	B	292	LEU
2	B	328	LYS
2	B	348	LEU
2	B	385	GLU
1	C	6	LYS
1	C	55	LEU
1	C	71[A]	HIS
1	C	71[B]	HIS
1	C	101	LEU
1	C	122	ARG
1	C	148	LEU
1	C	295	HIS
1	C	297	ARG

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Mol	Chain	Res	Type
2	D	199	TYR
2	D	232	LEU
2	D	283	ASP
2	D	284	ASP
2	D	292	LEU
2	D	328	LYS
2	D	348	LEU
2	D	378	GLN
2	D	433	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 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	TPO	A	160	1	10,10,11	6.02	1 (10%)	12,14,16	1.00	0
1	TPO	C	160	1	10,10,11	5.57	1 (10%)	12,14,16	0.93	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	TPO	A	160	1	-	0/9/11/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	C	160	1	-	0/9/11/13	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	O-C	18.89	1.24	1.11
1	C	160	TPO	O-C	17.46	1.23	1.11

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 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	#$|Z| > 2$
3	RRC	A	299	-	28,28,28	1.24	3 (10%)	38,38,38	3.13	14 (36%)
4	SGM	B	1	-	5,5,5	0.54	0	5,5,5	0.73	0
4	SGM	B	440	-	5,5,5	0.48	0	5,5,5	0.79	0
3	RRC	C	299	-	28,28,28	1.24	2 (7%)	38,38,38	3.27	13 (34%)
4	SGM	D	1	-	5,5,5	0.48	0	5,5,5	0.92	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
3	RRC	A	299	-	-	0/17/17/17	0/1/3/3
4	SGM	B	1	-	-	0/4/4/4	0/0/0/0
4	SGM	B	440	-	-	0/4/4/4	0/0/0/0
3	RRC	C	299	-	-	0/17/17/17	0/1/3/3
4	SGM	D	1	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	299	RRC	CAV-NAW	-4.60	1.31	1.37
3	A	299	RRC	CAV-NAW	-4.45	1.31	1.37
3	C	299	RRC	CAM-CAN	-2.42	1.39	1.44
3	A	299	RRC	CAM-CAN	-2.34	1.39	1.44
3	A	299	RRC	CAM-NAL	2.06	1.36	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	299	RRC	CAX-NAW-CAZ	11.71	137.40	125.43
3	A	299	RRC	CAX-NAW-CAZ	11.31	137.00	125.43
3	C	299	RRC	CAZ-NAW-CAV	-10.36	112.55	127.17
3	A	299	RRC	CAZ-NAW-CAV	-9.75	113.42	127.17
3	C	299	RRC	CBA-CAZ-NAW	7.62	122.24	110.33
3	A	299	RRC	CBA-CAZ-NAW	6.55	120.57	110.33
3	A	299	RRC	NAU-CAT-NAL	-3.91	120.16	126.19
3	C	299	RRC	CAX-NAW-CAV	3.82	109.81	106.90
3	C	299	RRC	NAU-CAT-NAL	-3.58	120.66	126.19
3	A	299	RRC	CAX-NAW-CAV	3.11	109.28	106.90
3	A	299	RRC	CAV-CAN-NAO	-3.02	106.93	109.52
3	C	299	RRC	CAV-CAN-NAO	-2.97	106.97	109.52
3	A	299	RRC	CAT-NAU-CAV	2.97	118.88	115.15
3	A	299	RRC	CAY-CAZ-NAW	2.52	114.27	110.33
3	C	299	RRC	NAO-CAX-NAW	-2.50	107.30	114.36
3	C	299	RRC	NAJ-CAM-NAL	2.49	121.50	118.76
3	C	299	RRC	CAT-NAU-CAV	2.45	118.22	115.15
3	C	299	RRC	CBA-CAZ-CAY	2.44	121.28	113.36
3	A	299	RRC	NAO-CAX-NAW	-2.44	107.47	114.36
3	C	299	RRC	NAS-CAT-NAU	2.42	120.31	116.94
3	A	299	RRC	CAT-NAL-CAM	2.36	121.87	116.97
3	C	299	RRC	CAT-NAL-CAM	2.32	121.79	116.97
3	A	299	RRC	CAN-CAV-NAU	-2.31	122.60	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	299	RRC	CAN-CAV-NAU	-2.30	122.62	125.94
3	A	299	RRC	CAD-NAJ-CAM	-2.29	120.22	123.22
3	A	299	RRC	NAS-CAT-NAU	2.15	119.93	116.94
3	A	299	RRC	NAS-CAT-NAL	2.13	119.91	116.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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 ⓘ

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	297/299 (99%)	0.12	19 (6%)	19	14	8, 16, 33, 45	0
1	C	267/299 (89%)	0.34	16 (5%)	21	16	14, 22, 39, 52	0
2	B	262/269 (97%)	0.11	13 (4%)	28	22	10, 19, 29, 40	0
2	D	269/269 (100%)	0.45	23 (8%)	11	7	11, 23, 38, 45	0
All	All	1095/1136 (96%)	0.25	71 (6%)	18	13	8, 20, 37, 52	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	LEU	6.7
2	D	433	HIS	6.7
1	C	295	HIS	6.7
2	D	432	VAL	6.0
2	D	284	ASP	5.8
2	B	284	ASP	5.3
2	D	434	HIS	5.3
2	B	432	VAL	5.2
1	C	253	PRO	5.2
2	B	323	GLN	5.0
1	A	97	THR	4.9
2	B	283	ASP	4.8
1	C	297	ARG	4.5
2	D	428	GLU	4.5
2	D	431	ASN	4.5
2	D	324	PRO	4.4
1	A	38	ASP	4.4
1	A	36	ARG	4.4
2	B	171	SER	4.3
1	A	71	HIS	4.3
1	C	296	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	71[A]	HIS	4.2
2	D	171	SER	4.1
2	D	378	GLN	4.1
1	C	287	GLN	3.9
1	A	41	THR	3.9
2	D	323	GLN	3.8
2	D	283	ASP	3.8
2	D	285	THR	3.8
1	A	74	ASN	3.7
1	A	73	GLU	3.5
2	B	280	TYR	3.5
1	C	162	GLU	3.4
2	B	428	GLU	3.4
1	A	72	THR	3.3
1	A	162[A]	GLU	3.2
1	C	219	LEU	3.2
1	C	269	TYR	3.1
2	D	280	TYR	3.0
1	C	36	ARG	2.9
1	C	73[A]	GLU	2.8
2	D	439	HIS	2.8
2	D	365	TYR	2.8
1	A	0	SER	2.8
2	B	431	ASN	2.7
1	A	37	LEU	2.5
2	D	419	HIS	2.5
1	A	206	ASP	2.5
1	C	293	VAL	2.5
1	C	216	PHE	2.5
1	C	282	ALA	2.4
1	C	2	GLU	2.3
2	D	400	ARG	2.3
2	B	285	THR	2.3
1	A	95	ALA	2.3
1	A	161	HIS	2.3
2	D	385	GLU	2.3
2	D	327	CYS	2.3
2	B	403	GLN	2.2
1	A	247	ASP	2.2
1	A	2	GLU	2.2
2	B	385	GLU	2.1
2	D	429	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	370	GLN	2.1
2	B	201	LYS	2.0
2	B	324	PRO	2.0
1	A	19	TYR	2.0
1	C	284	PRO	2.0
2	D	396	GLN	2.0
1	A	297	ARG	2.0
2	D	371	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	RSR	LLDF	B-factors($Å^2$)	Q<0.9
1	TPO	C	160	11/12	0.08	-0.62	16,19,23,23	0
1	TPO	A	160	11/12	0.06	-0.86	13,14,16,17	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors($Å^2$)	Q<0.9
4	SGM	B	440	6/6	0.41	15.47	41,41,42,44	0
4	SGM	D	1	6/6	0.41	6.46	42,44,45,51	0
4	SGM	B	1	6/6	0.36	4.34	39,40,41,43	0
3	RRC	C	299	26/26	0.15	1.03	16,18,23,24	0
3	RRC	A	299	26/26	0.15	0.66	14,16,21,22	0

6.5 Other polymers (i)

There are no such residues in this entry.