



wwPDB X-ray Structure Validation Summary Report

Oct 27, 2014 – 05:31 PM EDT

PDB ID : 4Q1F
Title : Human dCK C4S-S74E mutant in complex with UDP and the inhibitor 12R
{N-{2-[5-(4-{(1R)-1-[(4,6-diaminopyrimidin-2-yl)sulfanyl]ethyl}-5-methyl-1,3-thiazol-2-yl)-2-methoxyphenoxy]ethyl}methanesulfonamide}
Authors : Nomme, J.; Lavie, A.
Deposited on : 2014-04-03
Resolution : 2.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

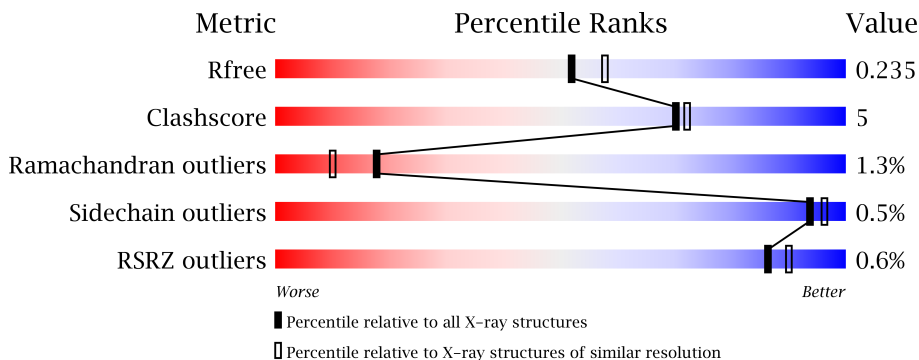
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance



The reported resolution of this entry is 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	280	
1	B	280	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4080 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 Deoxycytidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1897	1216	315	359	7			
1	B	231	Total	C	N	O	S	0	0	0
			1897	1216	315	359	7			

There are 50 discrepancies between the modelled and reference sequences:

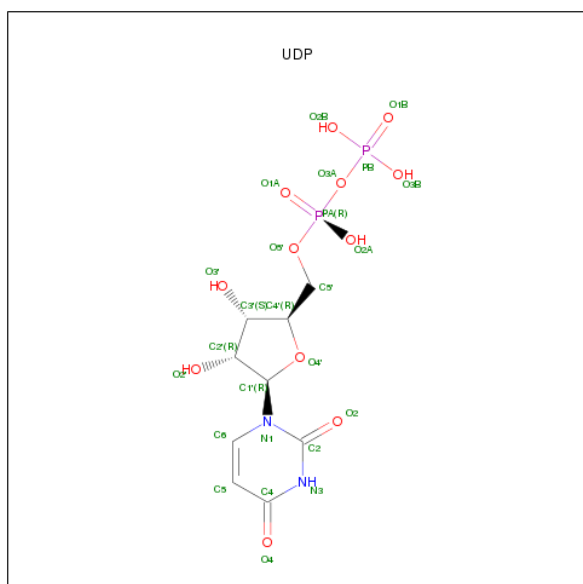
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P27707
A	-18	GLY	-	EXPRESSION TAG	UNP P27707
A	-17	SER	-	EXPRESSION TAG	UNP P27707
A	-16	SER	-	EXPRESSION TAG	UNP P27707
A	-15	HIS	-	EXPRESSION TAG	UNP P27707
A	-14	HIS	-	EXPRESSION TAG	UNP P27707
A	-13	HIS	-	EXPRESSION TAG	UNP P27707
A	-12	HIS	-	EXPRESSION TAG	UNP P27707
A	-11	HIS	-	EXPRESSION TAG	UNP P27707
A	-10	HIS	-	EXPRESSION TAG	UNP P27707
A	-9	SER	-	EXPRESSION TAG	UNP P27707
A	-8	SER	-	EXPRESSION TAG	UNP P27707
A	-7	GLY	-	EXPRESSION TAG	UNP P27707
A	-6	LEU	-	EXPRESSION TAG	UNP P27707
A	-5	VAL	-	EXPRESSION TAG	UNP P27707
A	-4	PRO	-	EXPRESSION TAG	UNP P27707
A	-3	ARG	-	EXPRESSION TAG	UNP P27707
A	-2	GLY	-	EXPRESSION TAG	UNP P27707
A	-1	SER	-	EXPRESSION TAG	UNP P27707
A	0	HIS	-	EXPRESSION TAG	UNP P27707
A	9	SER	CYS	ENGINEERED MUTATION	UNP P27707
A	45	SER	CYS	ENGINEERED MUTATION	UNP P27707
A	59	SER	CYS	ENGINEERED MUTATION	UNP P27707
A	74	GLU	SER	ENGINEERED MUTATION	UNP P27707
A	146	SER	CYS	ENGINEERED MUTATION	UNP P27707

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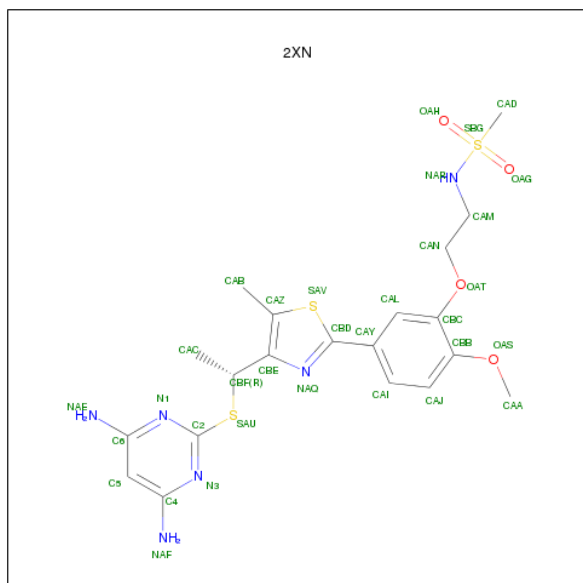
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP P27707
B	-18	GLY	-	EXPRESSION TAG	UNP P27707
B	-17	SER	-	EXPRESSION TAG	UNP P27707
B	-16	SER	-	EXPRESSION TAG	UNP P27707
B	-15	HIS	-	EXPRESSION TAG	UNP P27707
B	-14	HIS	-	EXPRESSION TAG	UNP P27707
B	-13	HIS	-	EXPRESSION TAG	UNP P27707
B	-12	HIS	-	EXPRESSION TAG	UNP P27707
B	-11	HIS	-	EXPRESSION TAG	UNP P27707
B	-10	HIS	-	EXPRESSION TAG	UNP P27707
B	-9	SER	-	EXPRESSION TAG	UNP P27707
B	-8	SER	-	EXPRESSION TAG	UNP P27707
B	-7	GLY	-	EXPRESSION TAG	UNP P27707
B	-6	LEU	-	EXPRESSION TAG	UNP P27707
B	-5	VAL	-	EXPRESSION TAG	UNP P27707
B	-4	PRO	-	EXPRESSION TAG	UNP P27707
B	-3	ARG	-	EXPRESSION TAG	UNP P27707
B	-2	GLY	-	EXPRESSION TAG	UNP P27707
B	-1	SER	-	EXPRESSION TAG	UNP P27707
B	0	HIS	-	EXPRESSION TAG	UNP P27707
B	9	SER	CYS	ENGINEERED MUTATION	UNP P27707
B	45	SER	CYS	ENGINEERED MUTATION	UNP P27707
B	59	SER	CYS	ENGINEERED MUTATION	UNP P27707
B	74	GLU	SER	ENGINEERED MUTATION	UNP P27707
B	146	SER	CYS	ENGINEERED MUTATION	UNP P27707

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 25	C 9	N 2	O 12	P 2	0	0
2	B	1	Total 25	C 9	N 2	O 12	P 2	0	0

- Molecule 3 is N-{2-[5-(4-{(1R)-1-[(4,6-DIAMINOPYRIMIDIN-2-YL)SULFANYL]ETHYL}-5-METHYL-1,3-THIAZOL-2-YL)-2-METHOXYPHENOXY]ETHYL}METHANESULFONAMIDE (three-letter code: 2XN) (formula: C₂₀H₂₆N₆O₄S₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 33	C 20	N 6	O 4	S 3	0	0
3	B	1	Total 33	C 20	N 6	O 4	S 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	82	Total O 82 82	0	0
4	B	88	Total O 88 88	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	68.78Å 68.78Å 121.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.43 – 2.10 27.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.8 (27.43-2.10) 97.8 (27.74-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.203 , 0.231 0.203 , 0.235	Depositor DCC
R_{free} test set	1647 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.8	EDS
Estimated twinning fraction	0.487 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 32814 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4080	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 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UDP, 2XN

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	0.31	1/1942 (0.1%)	0.55	2/2630 (0.1%)
1	B	0.24	0/1942	0.42	0/2630
All	All	0.27	1/3884 (0.0%)	0.49	2/5260 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	GLU	CD-OE1	6.62	1.32	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ARG	NE-CZ-NH1	-12.20	114.20	120.30
1	A	194	ARG	NE-CZ-NH2	8.62	124.61	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1897	0	1822	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1897	0	1822	14	0
2	A	25	0	11	0	0
2	B	25	0	11	1	0
3	A	33	0	0	0	0
3	B	33	0	0	0	0
4	A	82	0	0	1	0
4	B	88	0	0	1	0
All	All	4080	0	3666	35	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 5.

The worst 5 of 35 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:219:ARG:NH2	1:B:231:VAL:O	2.21	0.74
1:B:195:ASN:OD1	4:B:463:HOH:O	2.15	0.64
1:A:237:ASP:OD1	1:A:239:ASN:ND2	2.36	0.58
1:B:213:GLU:HG3	1:B:217:LEU:HB3	1.86	0.57
1:B:219:ARG:HE	1:B:233:ILE:HD12	1.70	0.54

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	227/280 (81%)	214 (94%)	10 (4%)	3 (1%)	18	10
1	B	227/280 (81%)	212 (93%)	12 (5%)	3 (1%)	18	10
All	All	454/560 (81%)	426 (94%)	22 (5%)	6 (1%)	18	10

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	ASN
1	A	198	GLN
1	B	196	GLU
1	A	166	PHE
1	A	194	ARG

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	204/256 (80%)	203 (100%)	1 (0%)	94	96
1	B	204/256 (80%)	203 (100%)	1 (0%)	94	96
All	All	408/512 (80%)	406 (100%)	2 (0%)	94	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	B	195	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	B	97	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	UDP	A	301	-	26,26,26	0.96	0	36,40,40	1.35	2 (5%)
3	2XN	A	302	-	35,35,35	3.09	10 (28%)	48,50,50	2.62	20 (41%)
2	UDP	B	301	-	26,26,26	0.93	0	36,40,40	1.37	2 (5%)
3	2XN	B	302	-	35,35,35	3.28	10 (28%)	48,50,50	2.77	18 (37%)

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	UDP	A	301	-	-	0/14/32/32	0/2/2/2
3	2XN	A	302	-	-	1/18/22/22	0/3/3/3
2	UDP	B	301	-	-	0/14/32/32	0/2/2/2
3	2XN	B	302	-	-	0/18/22/22	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	2XN	CAZ-SAV	-9.62	1.57	1.73
3	A	302	2XN	CAY-CBD	-9.60	1.33	1.46
3	B	302	2XN	CAY-CBD	-9.24	1.33	1.46
3	A	302	2XN	CAZ-SAV	-9.04	1.58	1.73
3	B	302	2XN	CBD-SAV	-7.49	1.63	1.73

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	2XN	CAA-OAS-CBB	8.98	130.83	117.56
3	A	302	2XN	CAA-OAS-CBB	7.64	128.86	117.56
3	B	302	2XN	OAS-CBB-CBC	6.32	124.51	115.41
3	B	302	2XN	OAG-SBG-OAH	-5.89	109.03	118.76
3	A	302	2XN	OAS-CBB-CBC	5.84	123.82	115.41

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	2XN	CAD-SBG-NAR-CAM

There are no ring outliers.

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 ⓘ

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	231/280 (82%)	0.07	2 (0%) 81 85	32, 46, 65, 83	1 (0%)
1	B	231/280 (82%)	0.08	1 (0%) 90 92	31, 46, 71, 83	1 (0%)
All	All	462/560 (82%)	0.08	3 (0%) 86 90	31, 46, 69, 83	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	PHE	3.9
1	A	197	GLU	2.4
1	A	166	PHE	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
3	2XN	B	302	33/33	0.14	0.22	37,47,81,96	0
3	2XN	A	302	33/33	0.12	-0.51	37,46,60,75	0
2	UDP	A	301	25/25	0.12	-0.67	35,51,56,58	0
2	UDP	B	301	25/25	0.10	-1.04	37,52,56,59	0

6.5 Other polymers

There are no such residues in this entry.